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(54) **Structure of a glucocorticoid receptor ligand binding domain comprising an expanded binding pocket and methods employing same**

(57) A solved three-dimensional crystal structure of a glucocorticoid receptor (GR) α ligand binding domain polypeptide is disclosed, in the form of a crystalline glucocorticoid receptor α ligand binding domain polypeptide in complex with the ligand fluticasone propionate (FP) and a peptide derived from the co-activator TIF2. The GR/FP/TIF2 structure includes an expanded binding pocket not seen in other GR structures. Methods of designing steroid and non-steroid modulators of the bi-

ological activity of GR and other nuclear receptors (NRs) are also disclosed. In another aspect of the present invention homology models of androgen receptor (AR), progesterone receptor (PR) and mineralcorticoid receptor (MR) are disclosed, as well as methods of forming homology models for other NRs. Methods of forming a soluble GR/FP/TIF2 complex are also disclosed.

Description

Technical Field

5 [0001] The present invention relates generally to a glucocorticoid receptor polypeptide, to a glucocorticoid receptor ligand binding domain polypeptide, and to the structure of a glucocorticoid receptor ligand binding domain bound to fluticasone propionate and a co-activator peptide. This structure reveals an expanded binding pocket having a configuration and volume not observed in other GR structures, which explains the observed binding of some ligands to GR. In one aspect, the invention relates to methods by which a soluble complex comprising glucocorticoid ligand binding domain, fluticasone propionate and a co-activator can be generated. Methods by which modulators and ligands of nuclear receptors, particularly steroid receptors, and more particularly glucocorticoid receptors, and the ligand binding domains thereof, can be identified are also disclosed. The invention further relates to homology models of nuclear receptors, preferably the ligand binding domains of nuclear receptors, which can be generated using the structure of a glucocorticoid receptor of the present invention, as well as docking models of an association between a ligand and a nuclear receptor.

Abbreviations	
ATP	adenosine triphosphate
ADP	adenosine diphosphate
APS	Advanced Photon Source
AR	androgen receptor
CAT	chloramphenicol acyltransferase
CCD	charge-coupled device
cDNA	complementary DNA
DBD	DNA binding domain
DEX	dexamethasone
DHT	dihydrotestosterone
DMSO	dimethyl sulfoxide
DNA	deoxyribonucleic acid
DTT	dithiothreitol
EDTA	ethylenediaminetetraacetic acid
ER	estrogen receptor
FP	fluticasone propionate
GR	glucocorticoid receptor
GR α	glucocorticoid receptor α
GRE	glucocorticoid responsive element
HEPES	N-2-hydroxyethylpiperazine-N'-2-ethanesulfonic acid
HSP	heat shock protein
kDa	kilodalton(s)
LBD	ligand binding domain
MM	molecular mechanics
MR	mineralocorticoid receptor
NDP	nucleotide diphosphate
NID	nuclear receptor interaction domain
NR	nuclear receptor
NTP	nucleotide triphosphate
PAGE	polyacrylamide gel electrophoresis
PCR	polymerase chain reaction
PG	progesterone
pI	isoelectric point
PPAR	peroxisome proliferator-activated receptor
PR	progesterone receptor
QSAR	quantitative structure-activity relationship

(continued)

Abbreviations	
RAR	retinoid acid receptor
RXR	retinoid X receptor
SAR	structure-activity relationship
SDS	sodium dodecyl sulfate
SDS-PAGE	sodium dodecyl sulfate polyacrylamide gel electrophoresis
SR	steroid receptor
TIF2	transcription intermediary factor 2
TR	thyroid receptor
VDR	vitamin D receptor

Amino Acid Abbreviations		
Single-Letter Code	Three-Letter Code	Name
A	Ala	Alanine
V	Val	Valine
L	Leu	Leucine
I	Ile	Isoleucine
P	Pro	Proline
F	Phe	Phenylalanine
W	Trp	Tryptophan
M	Met	Methionine
G	Gly	Glycine
S	Ser	Serine
T	Thr	Threonine
C	Cys	Cysteine
Y	Tyr	Tyrosine
N	Asn	Asparagine
Q	Gln	Glutamine
D	Asp	Aspartic Acid
E	Glu	Glutamic Acid
K	Lys	Lysine
R	Arg	Arginine
H	His	Histidine

Functionally Equivalent Codons

<u>Amino Acid</u>	<u>Codons</u>
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	Alanine	Ala	A	GCA GCC GCG GCU
5	Cysteine	Cys	C	UGC UGU
	Aspartic Acid	Asp	D	GAC GAU
	Glumatic acid	Glu	E	GAA GAG
10	Phenylalanine	Phe	F	UUC UUU
	Glycine	Gly	G	GGA GGC GGG GGU
	Histidine	His	H	CAC CAU
15	Isoleucine	Ile	I	AUA AUC AUU
	Lysine	Lys	K	AAA AAG
	Methionine	Met	M	AUG
20	Asparagine	Asn	N	AAC AAU
	Proline	Pro	P	CCA CCC CCG CCU
	Glutamine	Gln	Q	CAA CAG
25	Threonine	Thr	T	ACA ACC ACG ACU
	Valine	Val	V	GUA GUC GUG GUU
	Tryptophan	Trp	W	UGG
30	Tyrosine	Tyr	Y	UAC UAU
	Leucine	Leu	L	UUA UUG CUA CUC
				CUG CUU
35	Arginine	Arg	R	AGA AGG CGA CGC
				CGG CGU
40	Serine	Ser	S	ACG AGU UCA UCC
				UCG UCU

Background Art

[0002] Nuclear receptors represent a superfamily of proteins that specifically bind a physiologically relevant small molecule, such as a hormone or vitamin. As a result of a molecule binding to a nuclear receptor, the nuclear receptor changes the ability of a cell to transcribe DNA, i.e. nuclear receptors modulate the transcription of DNA. However, they can also have transcription independent actions.

[0003] Unlike integral membrane receptors and membrane-associated receptors, nuclear receptors reside in either the cytoplasm or nucleus of eukaryotic cells. Thus, nuclear receptors comprise a class of intracellular, soluble, ligand-regulated transcription factors. Nuclear receptors include but are not limited to receptors for androgens, mineralcorticoids, progestins, estrogens, thyroid hormones, vitamin D, retinoids, eicosanoids, peroxisome proliferators and, pertinently, glucocorticoids. Many nuclear receptors, identified by either sequence homology to known receptors (See, e.g., Drewes et al., (1996) *Mol. Cell. Biol.* 16:925-31) or based on their affinity for specific DNA binding sites in gene promoters (See, e.g., Sladek et al., *Genes Dev.* 4:2353-65), have unascertained ligands and are therefore commonly termed "orphan receptors."

[0004] Glucocorticoids are an example of a cellular molecule that has been associated with cellular proliferation.

Glucocorticoids are known to induce growth arrest in the G1-phase of the cell cycle in a variety of cells, both *in vivo* and *in vitro*, and have been shown to be useful in the treatment of certain cancers. The glucocorticoid receptor (GR) belongs to an important class of transcription factors that alter the expression of target genes in response to a specific hormone signal. Accumulated evidence indicates that receptor associated proteins play key roles in regulating glucocorticoid signaling. The list of cellular proteins that can bind and co-purify with the GR is constantly expanding.

[0005] Glucocorticoids are also used for their anti-inflammatory effect on the skin, joints, and tendons. They are important for treatment of disorders in which inflammation is thought to be caused by immune system activity. Representative disorders of this sort include but are not limited to rheumatoid arthritis, inflammatory bowel disease, glomerulonephritis, and connective tissue diseases like systemic lupus erythematosus. Glucocorticoids are also used to treat asthma (e.g. fluticasone propionate, a component of the asthma medication ADVAIR™ marketed by GlaxoSmithKline) and are widely used with other drugs to prevent the rejection of organ transplants. Some cancers of the blood (leukemias) and lymphatic system (lymphomas) can also respond to corticosteroid drugs.

[0006] Glucocorticoids exert several effects in tissues that express receptors for them. They regulate the expression of several genes either positively or negatively and in a direct or indirect manner. They are also known to arrest the growth of certain lymphoid cells and in some cases cause cell death (Harmon et al., (1979) *J. Cell Physiol.* 98: 267-278; Yamamoto, (1985) *Ann. Rev. Genet.* 19: 209-252; Evans, (1988) *Science* 240:889-895; Beato, (1989) *Cell* 56:335-344; Thompson, (1989) *Cancer Res.* 49: 2259s-2265s.). Due in part to their ability to kill cells, glucocorticoids have been used for decades in the treatment of leukemias, lymphomas, breast cancer, solid tumors and other diseases involving irregular cell growth, e.g. psoriasis. The inclusion of glucocorticoids in chemotherapeutic regimens has contributed to a high rate of cure of certain leukemias and lymphomas which were formerly lethal (Homo-Delarche, (1984) *Cancer Res.* 44: 431-437). Although it is clear that glucocorticoids exert these effects after binding to their receptors, the mechanism of killing cells is not completely understood, although several hypotheses have been proposed. Among the more prominent hypotheses are: the deinduction of critical lymphokines, oncogenes and growth factors; the induction of supposed "lysis genes;" alterations in calcium ion influx; the induction of endonucleases; and the induction of a cyclic AMP-dependent protein kinase (McConkey et al., (1989) *Arch. Biochem. Biophys.* 269: 365-370; Cohen & Duke, (1984) *J. Immunol.* 152: 38-42; Eastman-Reks & Vedeckis, (1986) *Cancer Res.* 46: 2457-2462; Kelso & Munck, (1984) *J. Immunol.* 133:784-791; Gruol et al., (1989) *Molec. Endocrinol.* 3: 2119-2127; Yuh & Thompson, (1989) *J. Biol. Chem.* 264: 10904-10910).

[0007] Fluticasone propionate (FP) is a corticosteroid that forms one active component of the GlaxoSmithKline product ADVAIR™, which is indicated for treatment of asthma. Fluticasone propionate is a GR modulator. As an asthma medicine, fluticasone propionate reduces swelling and inflammation inside the lungs of a patient. The precise mechanism of this effect is not presently known. Fluticasone propionate has been found to have an affinity for GR 18 times that of dexamethasone, another commonly employed corticosteroid. The present invention offers some insight into this observed pattern of affinity for GR.

[0008] Polypeptides, e.g. the glucocorticoid receptor ligand binding domain, have a three-dimensional structure determined by the primary amino acid sequence and the environment surrounding the polypeptide. This three-dimensional structure establishes the polypeptide's activity, stability, binding affinity, binding specificity, and other biochemical attributes. Thus, knowledge of a protein's three-dimensional structure can provide much guidance in designing agents that mimic, inhibit, or improve its biological activity.

[0009] The three-dimensional structure of a polypeptide can be determined in a number of ways. Many of the most precise methods employ X-ray crystallography (See, e.g., Van Holde, (1971) *Physical Biochemistry*, Prentice-Hall, New Jersey, pp. 221-39). This technique relies on the ability of crystalline lattices to diffract X-rays or other forms of radiation. Diffraction experiments suitable for determining the three-dimensional structure of macromolecules typically require high-quality crystals. Unfortunately, such crystals have been unavailable for the ligand binding domain of a human glucocorticoid receptor, as well as many other proteins of interest. Thus, high-quality diffracting crystals of the ligand binding domain of a human glucocorticoid receptor in complex with a ligand would greatly assist in the elucidation of its three-dimensional structure.

[0010] Clearly, the solved crystal structure of the ligand binding domain of a glucocorticoid receptor polypeptide in complex with a ligand and a co-activator peptide would be useful in the process of the rational design of modulators of activity mediated by the glucocorticoid receptor. Evaluation of the available sequence data shows that GR α is particularly similar to MR, PR and AR. The GR α LBD has approximately 56%, 54% and 50% sequence identity to the MR, PR and AR LBDs, respectively. The GR β amino acid sequence is identical to the GR α amino acid sequence for residues 1-727, but the remaining 15 residues in GR β show no significant similarity to the remaining 50 residues in GR α . If no X-ray structure were available for GR α , then one could build a model for GR α using the available X-ray structures of PR and/or AR as templates. These theoretical models have some utility, but cannot be as accurate as a true X-ray structure, such as the X-ray structure disclosed here. Because of their limited accuracy, a model for GR α will generally be less useful than an X-ray structure for the design of agonists, antagonists and modulators of GR α .

[0011] Additionally, a solved GR α -co-activator peptide-fluticasone propionate crystal structure would provide struc-

tural details and insights necessary to design a modulator of GR α that maximizes preferred requirements for any modulator, i.e. potency and specificity. By exploiting the structural details obtained from a GR α -co-activator peptide-fluticasone propionate crystal structure, it would be possible to design a GR α modulator that, despite GR α 's similarity with other steroid receptors and nuclear receptors, exploits the unique structural features of the ligand binding domain of human GR α . A GR α modulator developed using structure-assisted design would take advantage of heretofore unknown GR α structural considerations and thus be more effective than a modulator developed using homology-based design or other GR α structures. Potential or existent homology models or existing crystal structures cannot provide the necessary degree of specificity. A GR α modulator designed using the structural coordinates of a crystalline form of the ligand binding domain of GR α in complex with fluticasone propionate and a co-activator peptide would also provide a starting point for the development of modulators of other nuclear receptors.

[0012] Although several journal articles have referred to GR mutants having "increased ligand efficacy" in cell-based assays, it has not been mentioned that such mutants could have improved solution properties so that they could provide a suitable reagent for purification, assay, and crystallization. See Garabedian & Yamamoto, (1992) *Mol. Biol. Cell* 3: 1245-1257; Kralli et al., (1995) *Proc. Natl. Acad. Sci.* 92: 4701-4705; Bohen, (1995) *J. Biol. Chem.* 270: 29433-29438; Bohen, (1998) *Mol. Cell. Biol.* 18: 3330-3339; Freeman et al., (2000) *Genes Dev.* 14: 422-434.

[0013] Indeed, it is well documented that GR associates with molecular chaperones (e.g. heat shock proteins (HSPs) such as hsp90, hsc70, and p23). In the past, it has been considered that GR would either not be active or soluble if purified away from these binding partners. In fact, it has even been mentioned that GR must be in complex with hsp90 in order to adopt a high affinity steroid binding conformation. See Xu et al., (1998) *J. Biol. Chem.* 273: 13918-13924; Rajapandi et al., (2000) *J. Biol. Chem.* 275: 22597-22604.

[0014] Still other journal articles have reported *E.coli* expression of GST-GR, but also noted a failure to purify the purported polypeptide. See Ohara-Nemoto et al., (1990) *J. Steroid Biochem. Molec. Biol.* 37: 481-490; Caamano et al., (1994) *Annal. NYAcad. Sci.* 746: 68-77.

[0015] The structure of GR in complex with dexamethasone was previously solved ("the Dex structure"), the atomic coordinates of which are presented in Table 3. While offering unprecedented insight into the structure of GR in complex with a ligand, this structure does not adequately answer the question surrounding the higher affinity of GR for FP than for dexamethasone. Nor does the GR/Dex structure explain the structural requirements for association of FP with GR and other NRs. For example, examination of the GR/Dex structure initially suggests that the binding pocket of GR, AR, MR and PR is too small to accommodate the FP ligand. Nor can available GR, AR, MR and PR models adequately explain the mode of FP association with these NRs. Examination of these models indicates that the ligand binding pocket is sterically limited in its ability to accommodate FP and other ligands, such as steroidal molecules having large substituents at the C-17 α position and non-steroidal molecules having substituents predicted to fill the same space as would be filled by the propionate group of FP. These larger ligands, including FP, are nonetheless known to bind these NRs, presumably by expanding the ligand binding pocket in some way. Until the disclosure of the present invention, the details of this expansion, including the identity of movements of structural features of a GR protein, were not known, and would have been exceptionally difficult to predict with protein modelling software. A crystal structure of FP in complex with GR would provide insight into the binding of larger ligands to not only GR, but other NRs as well, including AR, MR and PR. Such a structure could also form a basis for the construction of homology models and docking models of these and other nuclear receptors.

[0016] Importantly, a GR/FP structure could be employed in modulator design. This structure would be particularly valuable because it would provide insight into the structural features of GR that are involved in binding FP. Since available structures and models cannot adequately account for the binding of FP and certain other ligands and in fact suggest that, based on a steric evaluation of the ligand-receptor interaction, such binding would not be likely to be productive, a solved structure of GR in complex with FP would be of particular value to researchers involved with the rational design of NR modulators, particularly modulators of GR, AR, PR and MR. Further, such a structure could form the basis of one or more homology models and docking models; these models would be particularly valuable since they would account for receptor-specific features that a general NR model could not. The generation of such models would be of assistance in designing receptor-specific modulators.

[0017] What is needed, therefore, is a purified, soluble GR α LBD polypeptide in complex with a steroidal ligand having a substituent larger than a hydroxyl group at the C17- α position, preferably also with a co-activator peptide, for use in structural studies, as well as methods for making the same. Such methods would also find application in the preparation of modified NRs in general.

[0018] What is also needed is a crystallized form of a GR α ligand binding domain, preferably in complex with fluticasone propionate and a co-activator peptide. Acquisition of crystals of the GR α ligand binding domain polypeptide in complex with fluticasone propionate and a co-activator peptide facilitates a determination of a three-dimensional structure of a GR α ligand binding domain (LBD) polypeptide in the conformation adopted by GR α when it binds fluticasone propionate and a co-activator peptide. Knowledge of this three dimensional structure can facilitate the design of modulators of GR-mediated activity. Such modulators can lead to therapeutic compounds to treat a wide range of conditions,

including inflammation, tissue rejection, auto-immunity, malignancies such as leukemias and lymphomas, Cushing's syndrome, acute adrenal insufficiency, congenital adrenal hyperplasia, rheumatic fever, polyarteritis nodosa, granulomatous polyarteritis, inhibition of myeloid cell lines, immune proliferation/apoptosis, HPA axis suppression and regulation, hypercortisolemia, modulation of the TH1/TH2 cytokine balance, chronic kidney disease, stroke and spinal cord injury, hypercalcemia, hyperglycemia, acute adrenal insufficiency, chronic primary adrenal insufficiency, secondary adrenal insufficiency, congenital adrenal hyperplasia, cerebral edema, thrombocytopenia, Little's syndrome, inflammatory bowel disease, systemic lupus erythematosus, polyarthritis nodosa, Wegener's granulomatosis, giant cell arteritis, rheumatoid arthritis, osteoarthritis, hay fever, allergic rhinitis, urticaria, angioneurotic edema, chronic obstructive pulmonary disease, asthma, tendonitis, bursitis, Crohn's disease, ulcerative colitis, autoimmune chronic active hepatitis, organ transplantation, hepatitis, cirrhosis, inflammatory scalp alopecia, panniculitis, psoriasis, discoid lupus erythematosus, inflamed cysts, atopic dermatitis, pyoderma gangrenosum, pemphigus vulgaris, bullous pemphigoid, systemic lupus erythematosus, dermatomyositis, herpes gestationis, eosinophilic fasciitis, relapsing polychondritis, inflammatory vasculitis, sarcoidosis, Sweet's disease, type 1 reactive leprosy, capillary hemangiomas, contact dermatitis, atopic dermatitis, lichen planus, exfoliative dermatitis, erythema nodosum, acne, hirsutism, toxic epidermal necrolysis, erythema multiform, cutaneous T-cell lymphoma. Other applications of a GR modulator developed in accordance with the present invention can be employed to treat Human Immunodeficiency Virus (HIV), cell apoptosis, and can be employed in treating cancerous conditions including, but not limited to, Kaposi's sarcoma, immune system activation and modulation, desensitization of inflammatory responses, IL-1 expression, natural killer cell development, lymphocytic leukemia, treatment of retinitis pigmentosa. Other applications for such a modulator comprise modulating cognitive performance, memory and learning enhancement, depression, addiction, mood disorders, chronic fatigue syndrome, schizophrenia, stroke, sleep disorders, anxiety, immunostimulants, repressors, wound healing and a role as a tissue repair agent or in anti-retroviral therapy.

Summary of the Invention

[0019] A crystalline GR polypeptide complex comprising an expanded binding pocket is disclosed. Preferably, the crystalline form has lattice constants of $a = b = 127.656 \text{ \AA}$, $c = 87.725 \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 120^\circ$. Preferably, the crystalline form is a hexagonal crystalline form. More preferably, the crystalline form has a space group of $P6_1$. Even more preferably, the GR ligand binding domain polypeptide comprises the amino acid sequence shown in SEQ ID NOs: 6 and 8. Even more preferably, the GR ligand binding domain has a crystalline structure further characterized by the coordinates corresponding to Table 2.

[0020] Preferably, the GR polypeptide complex comprises a ligand and a co-activator peptide. Optionally, the crystalline form contains two GR ligand binding domain polypeptides in the asymmetric unit. Preferably, the crystalline form is such that the three-dimensional structure of the crystallized GR ligand binding domain polypeptide can be determined to a resolution of about 3.0 \AA or better. Even more preferably, the crystalline form contains one or more atoms having a molecular weight of 40 grams/mol or greater.

[0021] A method for determining the three-dimensional structure of a crystallized GR polypeptide complex comprising an expanded binding pocket to a resolution of about 3.0 \AA or better is disclosed. In a preferred embodiment, the method comprises: (a) crystallizing a GR ligand binding domain polypeptide; and (b) analyzing the GR ligand binding domain polypeptide to determine the three-dimensional structure of the crystallized GR ligand binding domain polypeptide, whereby the three-dimensional structure of a crystallized GR polypeptide complex comprising an expanded binding pocket is determined to a resolution of about 3.0 \AA or better.

[0022] Preferably, the complex comprises a ligand, preferably fluticasone propionate, and a co-activator peptide, preferably a TIF2 peptide. It is also preferable that the GR ligand binding domain polypeptide comprises the amino acid sequence of SEQ ID NOs: 6 and 8, and that the TIF2 peptide comprises SEQ ID NO: 9. Even more preferably, the three-dimensional structure is further characterized by the coordinates corresponding to Table 2.

[0023] A method of generating a crystallized GR polypeptide complex comprising an expanded binding pocket and a ligand known or suspected to be unable to associate with a known GR structure is disclosed. In a preferred embodiment, the method comprises: (a) providing a solution comprising a GR polypeptide and a ligand known or suspected to be unable to associate with a known GR structure; and (b) crystallizing the GR ligand binding domain polypeptide using the hanging drop method, whereby a crystallized GR polypeptide complex comprising an expanded binding pocket and a ligand known or suspected to be unable to associate with a known GR structure is generated.

[0024] Preferably, the complex comprises a ligand, preferably fluticasone propionate, and a co-activator peptide, preferably a TIF2 peptide. It is also preferable that the GR ligand binding domain polypeptide comprises the amino acid sequence of SEQ ID NOs: 6 or 8, and that the TIF2 peptide comprises SEQ ID NO: 9. Even more preferably, the complex is further characterized by the coordinates corresponding to Table 2.

[0025] A method for identifying a GR modulator is disclosed. In a preferred embodiment, the method comprises: (a) providing atomic coordinates of a GR polypeptide complex comprising an expanded binding pocket to a computerized

modeling system; and (b) modeling a ligand that fits spatially into the large pocket volume of the GR polypeptide complex to thereby identify a GR modulator.

[0026] Preferably, the complex comprises a ligand, preferably fluticasone propionate, and a co-activator peptide, preferably a TIF2 peptide. It is also preferable that the GR polypeptide comprises the amino acid sequence of SEQ ID NOs: 6 or 8, and that the TIF2 peptide comprises SEQ ID NO: 9. Even more preferably, the complex is further characterized by the coordinates corresponding to Table 2.

[0027] A method of designing a modulator that selectively modulates the activity of a GR α polypeptide comprising an expanded binding pocket is disclosed. In a preferred embodiment, the method comprises: (a) providing a crystalline form of a GR α polypeptide complex comprising an expanded binding pocket; (b) determining the three-dimensional structure of the crystalline form of the GR α ligand binding domain polypeptide; and (c) synthesizing a modulator based on the three-dimensional structure of the crystalline form of the GR α ligand binding domain polypeptide, whereby a modulator that selectively modulates the activity of a GR α polypeptide comprising an expanded binding pocket is designed.

[0028] Preferably, the complex comprises a ligand, preferably fluticasone propionate, and a co-activator peptide, preferably a TIF2 peptide. It is also preferable that the GR ligand binding domain polypeptide comprises the amino acid sequence of SEQ ID NOs: 6 or 8, and that the TIF2 peptide comprises SEQ ID NO: 9. Even more preferably, the three-dimensional structure is further characterized by the coordinates corresponding to Table 2.

[0029] A method of forming a homology model of an NR is disclosed. In a preferred embodiment, the method comprises: (a) providing a template amino acid sequence comprising a GR polypeptide comprising an expanded binding pocket; (b) providing a target NR amino acid sequence; (c) aligning the target sequence and the template sequence to form a homology model.

[0030] Preferably, the GR polypeptide comprises the amino acid sequence of SEQ ID NOs: 6 or 8, and that the TIF2 peptide comprises SEQ ID NO: 9.

[0031] A method of designing a modulator of a nuclear receptor is disclosed. In a preferred embodiment, the method comprises: (a) designing a potential modulator of a nuclear receptor that will make interactions with amino acids in the ligand binding site of the nuclear receptor based upon atomic structure coordinates of a NR polypeptide complex comprising an expanded binding pocket; (b) synthesizing the modulator; and (c) determining whether the potential modulator modulates the activity of the nuclear receptor, whereby a modulator of a nuclear receptor is designed.

[0032] Preferably, the complex comprises a ligand, preferably fluticasone propionate, and a co-activator peptide, preferably a TIF2 peptide. It is also preferable that the NR polypeptide comprises the amino acid sequence of SEQ ID NOs: 6 or 8, and that the TIF2 peptide comprises SEQ ID NO: 9. Even more preferably, the atomic structural coordinates are further characterized by the coordinates corresponding to Table 2.

[0033] A method of modeling an interaction between an NR and a non-steroid ligand is disclosed. In a preferred embodiment, the method comprises: (a) providing a homology model of a target NR generated using a crystalline GR polypeptide complex comprising an expanded binding pocket; (b) providing atomic coordinates of a non-steroid ligand; and (c) docking the non-steroid ligand with the homology model to form a NR/ligand model.

[0034] Preferably, the complex comprises a ligand, preferably fluticasone propionate, and a co-activator peptide, preferably a TIF2 peptide. It is also preferable that the GR polypeptide comprises the amino acid sequence of SEQ ID NOs: 6 or 8, and that the TIF2 peptide comprises SEQ ID NO: 9. Even more preferably, the complex is further characterized by the coordinates corresponding to Table 2.

[0035] A method of designing a non-steroid modulator of a target NR using a homology model is disclosed. In a preferred embodiment, the method comprises: (a) modeling an interaction between a target NR and a non-steroid ligand using a homology model generated using a crystalline GR polypeptide complex comprising an expanded binding pocket; (b) evaluating the interaction between the target NR and the non-steroid ligand to determine a first binding efficiency; (c) modifying the structure of the non-steroid ligand to form a modified ligand; (d) modeling an interaction between the modified ligand and the target NR; (e) evaluating the interaction between the target NR and the modified ligand to determine a second binding efficiency; and (f) repeating steps (c)-(e) a desired number of times if the second binding efficiency is less than the first binding efficiency.

[0036] Preferably, the complex comprises a ligand, preferably fluticasone propionate, and a co-activator peptide, preferably a TIF2 peptide. It is also preferable that the GR polypeptide comprises the amino acid sequence of SEQ ID NOs: 6 or 8, and that the TIF2 peptide comprises SEQ ID NO: 9. Even more preferably, the complex is further characterized by the coordinates corresponding to Table 2.

[0037] A data structure embodied in a computer-readable medium is disclosed. In a preferred embodiment, the data structure comprises: a first data field containing data representing spatial coordinates of an NR LBD comprising an expanded binding pocket, wherein the first data field is derived by combining at least a part of a second data field with at least a part of a third data field, and wherein (a) the second data field contains data representing spatial coordinates of the atoms comprising a GR LBD comprising an expanded binding pocket in complex with a ligand; and (b) the third data field contains data representing spatial coordinates of the atoms comprising a NR LBD. Preferably, the data of

the third data field comprises data selected from the data embodied in one of Table 3, Table 8, Table 9 and Table 10. It is also preferable that the GR LBD comprises the amino acid sequence of SEQ ID NOs: 6 or 8, and that the TIF2 peptide comprises SEQ ID NO: 9. Even more preferably, the complex is further characterized by the coordinates corresponding to Table 2.

[0038] A method for designing a homology model of the ligand binding domain of an NR wherein the homology model may be displayed as a three-dimensional image. In a preferred embodiment, the method comprises: (a) providing an amino acid sequence and an crystallographic structure of the ligand binding domain of a GR α polypeptide, (b) modifying said crystallographic structure to take account of differences between the amino acid configuration of the ligand binding domains of the NR on the one hand and the GR α polypeptide on the other hand, (c) verifying the accuracy of the homology model by comparing it with experimentally-determined NR protein and ligand properties, and if required, modifying the homology model for greater consistency with those binding properties.

[0039] A computational method of iteratively generating a homology model of the ligand binding domain of an NR, wherein the homology model is capable of being displayed as a three-dimensional image is disclosed. In a preferred embodiment, the method comprises: (a) entering into a computer a machine readable representation of an amino acid sequence of a ligand binding domain of a target NR polypeptide and a machine readable representation of a crystallographic structure of a ligand binding domain of a GR α polypeptide; (b) identifying a difference between an amino acid configuration of a ligand binding domain of a target NR and a GR α polypeptide; (c) modifying the machine readable representation of the crystallographic structure based on a difference identified in step (b) to thereby form a modified crystallographic structure; (d) comparing the modified crystallographic structure with an experimentally-determined property of one of the target NR and a ligand of the target NR; and (e) repeating steps (b) and (d) a desired number of times.

[0040] Accordingly, it is an object of the present invention to provide a three dimensional structure of the ligand binding domain of a GR. The object is achieved in whole or in part by the present invention.

[0041] An object of the invention having been stated hereinabove, other objects will be evident as the description proceeds, when taken in connection with the accompanying Drawings and Laboratory Examples as best described hereinbelow.

Brief Description of the Drawings

[0042]

Figure 1 is an autoradiogram of a polyacrylamide gel depicting the isolation of a GR mutant of the present invention. In this figure, Lane 1 contains the insoluble pellet fraction. Lane 2 contains the soluble supernatant fraction. Lane 3 contains pooled eluent from the initial Ni²⁺ column. Lane 4 contains the sample after thrombin digestion. Lane 5 contains the flow through fraction after reload of the Ni²⁺ column. Lane 6 contains the protein after anion exchange. The positions of molecular mass (kDa) markers are indicated on the left side of the figure. Figure 2 is a ribbon diagram showing an overview of the GR/TIF2/FP dimer complex. The ribbon representation of the two GR LBD is shown with gray and white, respectively, with the N-terminus and the C-terminus of the protein indicated. The fluticasone propionate molecules (FP) and TIF2 coactivator motifs are also identified.

Figure 3 is an electron density map (gray net) for the FP ligand and the surrounding residues (white sticks). The map was calculated with the 2Fo-Fc coefficient and is shown with 1 sigma cutoff. The propionate group of the FP molecule is also indicated.

Figure 4 is a ribbon diagram depicting the superposition of the GR/TIF2/FP and the GR/TIF2/Dex structures and showing the expanded binding pocket formed by rearrangement of helices 3, 6, 7 and 10, and the loop preceeding the AF-2 helix. Arrows indicate structural changes that expand the GR pocket to form an expanded binding pocket.

Figure 5A is a cartoon showing a semi-transparent surface representing the available pocket volume in GR subunit A in the GR/TIF2/Dex structure. Residues that surround the pocket are also presented.

Figure 5B is a cartoon showing a semi-transparent surface representing the available pocket volume in GR subunit B in the GR/TIF2/Dex structure. Residues that surround the pocket are also presented.

Figure 6A is a cartoon showing the expanded ligand-binding pocket of GR subunit A in the GR/TIF2/FP structure by a semi-transparent surface representing the available pocket volume. Residues that surround the pocket are also presented.

Figure 6B is a cartoon showing the expanded ligand-binding pocket of GR subunit B in the GR/TIF2/FP structure by a semi-transparent surface representing the available pocket volume. Residues that surround the pocket are also presented.

Figure 7A is a cartoon that uses a semi-transparent surface to show the extra pocket volume that is available to a ligand in the GR/TIF2/FP structure but is not available in the GR/TIF2/Dex structure. Residues around the pocket are also shown. In this figure GR subunit A is depicted.

Figure 7B is a cartoon that uses a semi-transparent surface to show the extra pocket volume that is available to a ligand in the GR/TIF2/FP structure but not available in the GR/TIF2/Dex structure. The surface was generated in the same manner as in Figure 7A. Key residues around the pocket are also shown. In this figure GR subunit B is depicted.

Figure 8A is a schematic representation of molecular interactions between the bound FP ligand and residues in subunit A of the GR protein. The dashed lines depict some of the significant interactions of 5.0 angstroms or less, although several less important interactions have been omitted for clarity.

Figure 8B is a schematic representation of molecular interactions between the bound FP ligand and residues in subunit B of the GR protein. The dashed lines depict some of the significant interactions of 5.0 angstroms or less, although several less important interactions have been omitted for clarity.

Figure 9 is a docking model of the Schering ligand, benzoxazin-1-one, bound to a GR LBD model derived from the GR/TIF2/FP crystal structure. The ligand is shown with a CPK drawing.

Figure 10 is a stick drawing of the ligand binding pocket of the GR structural model showing various interactions between the benzoxazin-1-one ligand and the amino acid residues that comprise the binding pocket.

Figure 11 is an orthogonal view of Figure 9 and illustrates the fitting of the *p*-fluorophenolic side chain of the benzoxazin-1-one into the expanded binding pocket of the GR structural model.

Figure 12 is a depiction of the overlay of the GR/TIF2/Dex crystal structure (grey) with the GR/benzoxazin-1-one model (white) comparing the geometries of the ligands and the relative locations of the amino acid side chains that comprise the GR expanded binding pocket.

Figure 13 is a docking model of the A-222977 ligand bound to a GR LBD model generated using the GR/TIF2/FP crystal structure. The ligand is shown as a CPK drawing.

Figure 14 is a stick drawing of the ligand binding pocket of the GR structural model showing key interactions between A-222977 and the amino acid residues that comprise the binding pocket.

Figure 15 is an orthogonal view of Figure 13 and illustrates the protrusion of methyl-sulfonyl-methoxyl-phenyl side chain of A-222977 into the expanded binding pocket of the GR structural model.

Figure 16 is a depiction of the overlay of the GR/Dex crystal structure (grey) with the GR/A-222977 (white) comparing the geometries of the ligands and the relative locations of the amino acid side chains that comprise the GR expanded binding pocket. Figure 17 is a sequence alignment of amino acid residues comprising the ligand binding domains of GR, MR, PR and AR.

Figure 18A is a ribbon drawing depicting the AR LBD homology model derived from the GR/TIF2/FP crystal structure.

Figure 18B is a ribbon diagram depicting a known AR/DHT LBD crystal structure; the ligand binding pocket, rendered as a solid surface, reveals no additional volume and no expanded binding pocket.

Figure 19 is a ribbon drawing of a docking model of bicalutamide bound to the LBD of the AR homology model derived from the GR/TIF2/FP crystal structure. The ligand is shown in a CPK drawing.

Figure 20 is an orthogonal view of the structure depicted in Figure 18A and shows the LBD of the AR homology model in complex with bicalutamide.

Figure 21 is a stick drawing of the ligand binding pocket of the AR homology model showing interactions between bicalutamide and the amino acid residues that comprise the binding pocket.

Figure 22 is an orthogonal view of Figure 20 and illustrates the protrusion of the *p*-fluorophenyl group of bicalutamide into the expanded binding pocket of the AR homology model.

Figure 23A is a ribbon drawing depicting the PR LBD homology model derived from the GR/TIF2/FP crystal structure; the PR ligand binding pocket, which is rendered as a solid surface, comprises an additional extension, similar to the additional volume of the GR expanded binding pocket.

Figure 23B is a ribbon diagram depicting a known PR/PG LBD crystal structure; the ligand binding pocket, rendered as a solid surface, reveals no expanded binding pocket.

Figure 24 is a ribbon drawing of a docking model of RWJ-60130 bound to the LBD of the PR homology model derived from the GR/TIF2/FP crystal structure. The ligand is shown in a CPK drawing.

Figure 25 is an orthogonal view of Figure 23 showing the LBD of the PR homology model bound with RWJ-60130.

Figure 26 is a stick drawing of the ligand binding pocket of the PR homology model showing interactions between RWJ-60130 and the amino acid residues that comprise the binding pocket.

Figure 27 is an orthogonal view of Figure 25 and illustrates the protrusion of the *p*-iodophenyl group of RWJ-60130 into the expanded binding pocket of the PR homology model.

Figure 28A is a ribbon drawing depicting an MR LBD homology model derived from the GR/TIF2/FP crystal structure; the MR ligand binding pocket, which is rendered as a solid surface, contains an additional extension, similar to that found in the GR expanded binding pocket.

Figure 28B is a ribbon drawing depicting an MR LBD homology model derived from the GR/TIF2/FP crystal structure; the PR ligand binding pocket, which is rendered as a solid surface, contains a smaller side pocket, similar to

the GR/Dex ligand binding pocket, which does not show the presence of an expanded binding pocket.

Brief Description of Sequences in the Sequence Listing

- 5 [0043] SEQ ID NOs: 1 and 2 are, respectively, a DNA sequence encoding a wild type full-length human glucocorticoid receptor (GenBank Accession No. 31679) and the amino acid sequence (GenBank Accession No. 121069) of a human glucocorticoid receptor encoded by the DNA sequence.
- [0044] SEQ ID NOs: 3 and 4 are, respectively, a DNA sequence encoding a F602S full-length human glucocorticoid receptor and the amino acid sequence of a human glucocorticoid receptor encoded by the DNA sequence.
- 10 [0045] SEQ ID NOs: 5 and 6 are, respectively, a DNA sequence encoding a wild type ligand binding domain of a human glucocorticoid receptor and the amino acid sequence of a human glucocorticoid receptor encoded by the DNA sequence.
- [0046] SEQ ID NOs: 7 and 8 are, respectively, a DNA sequence encoding a ligand binding domain (residues 521-777) of a human glucocorticoid receptor containing a phenylalanine to serine mutation at residue 602 and the amino acid
- 15 sequence of a human glucocorticoid receptor encoded by the DNA sequence.
- [0047] SEQ ID NO: 9 is an amino acid sequence of amino acid residues 740-753 of the human TIF2 protein.
- [0048] SEQ ID NO: 10 is an LXXLL motif of a human TIF2 protein.
- [0049] SEQ ID NO: 11 is an LLRYLL motif of a human TIF2 protein.

20 Detailed Description of the Invention

[0050] The present invention discloses a crystal structure of a ligand binding domain of GR in complex with a fluticasone propionate ligand and a peptide derived from the co-activator TIF2. This structure reveals an expanded binding pocket comprising additional volume that accommodates the propionate moiety of the FP ligand. The presence of this

25 additional volume is not observed in previous known GR/ligand structures, such as the structure of GR in complex with dexamethasone (characterized by the atomic coordinates of Table 3). The presence of the additional volume in the ligand binding pocket, which contributes to an "expanded binding pocket," accounts for observed ligand binding modes and can form the basis of homology models of GR and other nuclear receptors, including an androgen receptor, a progesterone receptor and a mineralocorticoid receptor. These homology models also form aspects of the present invention. Additionally, the expanded binding pocket can contribute to docking models that can be employed to understand and clarify the binding of a ligand to a nuclear receptor. Such homology and docking models can be employed

30 in the design of nuclear receptor modulators.

[0051] The present invention provides for the generation of a complex comprising a soluble GR LBD bound to fluticasone propionate and a TIF2 co-activator peptide. The present invention also provides for the ability to crystallize the

35 above complex and to determine its crystal structure. The GR LBD employed in the present invention comprises a single F602S mutation at residue 602. Thus, an aspect of the present invention comprises the use of both targeted and random mutagenesis of the GR gene to produce a recombinant protein with improved solution characteristics for the purposes of, for example, crystallization, characterization of biologically relevant protein-protein interactions, and compound screening assays. The present invention, which relates to GR LBD mutation F602S as well as other LBD mutations, demonstrates that GR can be overexpressed using an *E.coli* expression system and that active GR protein can be purified, assayed, and crystallized.

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[0052] Until disclosure of the present invention presented herein, the ability to obtain crystalline forms of the ligand binding domain of GR (e.g. GR α) in complex with fluticasone propionate and a co-activator peptide has not been realized. And until disclosure of the present invention presented herein, a detailed three-dimensional crystal structure

45 of a GR α LBD polypeptide in complex with fluticasone propionate and a co-activator peptide has not been solved. Moreover, nuclear receptor structures known in the art do not comprise an expanded binding pocket and therefore cannot fully explain the observed binding of some known ligands to various NRs.

[0053] In another aspect, the present invention provides for the generation of NR, SR and GR polypeptides and NR, SR or GR mutants (preferably GR α and GR α LBD mutants), and the ability to solve the crystal structures of those that crystallize. Indeed, a GR α LBD having a point mutation was crystallized and solved in one aspect of the present invention. Thus, an aspect of the present invention involves the use of both targeted and random mutagenesis of the

50 GR gene for the production of a recombinant protein with improved solution characteristics for the purpose of crystallization, characterization of biologically relevant protein-protein interactions, and compound screening assays. The present invention, relating to GR LBD F602S and other LBD mutations, shows that GR can be overexpressed using an *E.coli* expression system and that active GR protein can be purified, assayed, and crystallized.

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[0054] In addition to providing structural information, crystalline polypeptides provide other advantages. For example, the crystallization process itself further purifies the polypeptide, and satisfies one of the classical criteria for homogeneity. In fact, crystallization frequently provides unparalleled purification quality, removing impurities that are not re-

moved by other purification methods such as HPLC, dialysis, conventional column chromatography, and other methods. Moreover, crystalline polypeptides are sometimes stable at ambient temperatures and free of protease contamination and other degradation associated with solution storage. Crystalline polypeptides can also be useful as pharmaceutical preparations. Finally, crystallization techniques in general are largely free of problems such as denaturation associated with other stabilization methods (e.g., lyophilization). Once crystallization has been accomplished, crystallographic data provides useful structural information that can assist the design of compounds that can serve as modulators (e.g. agonists or antagonists), as described herein below. In addition, the crystal structure provides information useful to map a ligand binding site, which can then be mimicked by a chemical entity that can serve as an antagonist or agonist.

I. Definitions

[0055] Following long-standing patent law convention, the terms "a" and "an" mean "one or more" when used in this application, including the claims.

[0056] As used herein, the term "about," when referring to a value or to an amount of mass, weight, time, volume, concentration or percentage is meant to encompass variations of $\pm 20\%$ or $\pm 10\%$, more preferably $\pm 5\%$, even more preferably $\pm 1\%$, and still more preferably $\pm 0.1\%$ from the specified amount, as such variations are appropriate to perform the disclosed method.

[0057] As used herein, the terms "active position of the AF2 helix" and "active conformation of the AF2 helix" are used interchangeably and mean an AF2 helix having a position and/or orientation similar to that of an AF2 helix in a GR/TIF2/FP structure (e.g. as characterized by the atomic structural coordinates of Table 2), or similar to that of an AF2 helix in a GR/TIF2/Dex structure (e.g. as characterized by the atomic structural coordinates of Table 3). For example, with respect to GR, the "active position" is further characterized in GR by contacts between Leu757 in the AF2 helix and Trp600, Cys736, Phe737 and Phe740 in helices 5, 11, 11 and 11, respectively. The position and/or orientation of an AF2 helix in a structure comprising GR can be compared with that of an AF2 helix in a structure comprising a GR/FP complex by rotating and/or translating the GR structure so as to superimpose the backbone atoms of helices 1 through 10 onto the corresponding backbone atoms of helices 1 through 10 of a GR/TIF2/FP structure. A similar procedure can be employed to compare a structure of GR with that of another nuclear receptor, such as ER α or ER β . If, after superimposition, a majority of the backbone atoms of the core of the AF2 helix of the GR structure, (e.g. residues 752-757), lie within 1.0 angstroms of the position of corresponding backbone atoms of the AF2 helix of the GR/FP structure, then the AF2 helix is defined as being in an active position or active conformation. If more than half of the atoms lie more than 1.0 angstroms from their counterparts in the GR/FP structure, then the AF2 helix is considered to be in a position or conformation different from the active position or conformation.

[0058] In some cases, the AF2 helix might be disordered, or dynamically mobile. If several of the backbone atoms of the AF2 helix residues 752-757 are disordered so that they are not clearly defined in the electron density of an X-ray crystallographic experiment, then the AF2 helix as a whole is defined as assuming multiple positions and/or conformations. This ensemble of alternative positions or conformations might include positions or conformations that could be characterized as "active positions" or "active conformations." However, the disorder indicates that the "active position" or "active conformation" does not constitute an adequate fraction of the ensemble, and in this case the AF2 helix cannot be considered to be in the "active position" or "active conformation".

[0059] Other examples of a nuclear receptor where the AF2 helix is in an "active position" include the X-ray structures of the estrogen receptor α (ER α) bound to estradiol (Brzozowski et al., (1997) *Nature* 389:753) and diethylstilbestrol (DES) (Shiau et al., (1998) *Cell* 95:927). Examples of a nuclear receptor where the AF2 helix is not in an "active position" are the X-ray structures of the estrogen receptor α (ER α) bound to raloxifene (Brzozowski et al., (1997) *Nature* 389:753) and tamoxifen (Shiau et al., (1998) *Cell* 95:927). Binding of coactivator, and AF2-dependent activation of gene transcription, normally requires that the AF2 helix be in the "active position" (Nolte et al., (1998) *Nature* 395:137; Shiau et al., (1998) *Cell* 95:927). This creates a "charge-clamp" structure that holds the coactivator in its required position (Nolte et al., (1998) *Nature* 395:137). GR antagonists, such as RU-486, would be expected to displace the AF2 helix out of the "active position" and into some other position, such as the coactivator binding site as seen with raloxifene and tamoxifen in ER α (Brzozowski et al., (1997) *Nature* 389:753; Shiau et al., (1998) *Cell* 95:927).

[0060] The movement of the AF2 helix often induces other conformational changes in the protein that might not be compatible with agonist binding or activation of transcription. Also, the movement of the AF2 helix leaves the ligand binding pocket open to the exterior of the protein. These conformational modifications can make the structure unsuitable for structure-based design and docking calculations where the goal is the design of agonists or modulators where the protein remains predominantly in or near the active conformation.

[0061] As used herein, the term "agonist" means an agent that supplements or potentiates the bioactivity of a functional gene or protein or of a polypeptide encoded by a gene that is up- or down-regulated by a polypeptide and/or a polypeptide encoded by a gene that contains a binding site or response element in its promoter region. By way of specific example, an "agonist" is a compound that interacts with the steroid hormone receptor to promote a transcrip-

tional response. An agonist can induce changes in a receptor that places the receptor in an active conformation that allows them to influence transcription, either positively or negatively. There can be several different ligand-induced changes in the receptor's conformation. The term "agonist" specifically encompasses partial agonists.

[0062] As used herein, the terms " α -helix", "alpha-helix" and "alpha helix" are used interchangeably and mean the conformation of a polypeptide chain wherein the polypeptide backbone is wound around the long axis of the molecule in a left-handed or right-handed direction, and the R groups of the amino acids protrude outward from the helical backbone, wherein the repeating unit of the structure is a single turn of the helix, which extends about 0.56 nm along the long axis.

[0063] As used herein, the term "antagonist" means an agent that decreases or inhibits the bioactivity of a functional gene or protein, or that decrease or inhibit the bioactivity of a naturally occurring or engineered non-functional gene or protein. Alternatively, an antagonist can decrease or inhibit the bioactivity of a functional gene or polypeptide encoded by a gene that is up- or down-regulated by a polypeptide and/or contains a binding site or response element in its promoter region. An antagonist can also decrease or inhibit the bioactivity of a naturally occurring or engineered non-functional gene or polypeptide encoded by a gene that is up- or down-regulated by a polypeptide, and/or contains a binding site or response element in its promoter region. By way of specific example, an "antagonist" is a compound that interacts with the steroid hormone receptor to inhibit a transcriptional response. An antagonist can bind to a receptor but fail to induce conformational changes that alter the receptor's transcriptional regulatory properties or physiologically relevant conformations. Binding of an antagonist can also block the binding and therefore the actions of an agonist. The term "antagonist" specifically encompasses partial antagonists.

[0064] As used herein, the terms "backbone" and "backbone atoms" are the N, Ca, C and O atoms of a protein that are common to all twenty of the amino acids normally present in a protein. See G. E. Schulz and R. H. Schirmer, Principles of Protein Structure, Springer-Verlag, New York.

[0065] As used herein, the terms " β -sheet", "beta-sheet" and "beta sheet" are used interchangeably and mean the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

[0066] As used herein, the terms "binding pocket of an NR ligand binding domain", "NR ligand binding pocket," "NR ligand binding pocket" and "NR binding pocket" are used interchangeably, and refer to the large cavity within the NR ligand binding domain where a ligand can bind. This cavity can be empty, or can contain water molecules or other molecules from the solvent, or can contain ligand atoms. The binding pocket includes regions of space near the "main" binding pocket that not occupied by atoms of the NR but that are near the "main" binding pocket, and that are contiguous with the "main" binding pocket. For GR, the main binding pocket comprises the region of space encompassed by the residues shown in Figure 8.

[0067] As used herein, the term "biological activity" means any observable effect flowing from interaction between an NR (preferably a GR) polypeptide and a ligand. Representative, but non-limiting, examples of biological activity in the context of the present invention include transcription regulation, ligand binding and peptide binding.

[0068] As used herein, the terms "candidate substance" and "candidate compound" are used interchangeably and refer to a substance that is believed to interact with another moiety, for example a given ligand that is believed to interact with a complete target NR (preferably a GR) polypeptide or fragment thereof, and which can be subsequently evaluated for such an interaction. Representative candidate substances or compounds include xenobiotics such as drugs and other therapeutic agents, carcinogens and environmental pollutants, natural products and extracts, as well as endobiotics such as glucocorticosteroids, steroids, fatty acids and prostaglandins. Other examples of candidate compounds that can be investigated using the methods of the present invention include, but are not restricted to, agonists and antagonists of a GR polypeptide or other polypeptide, toxins and venoms, viral epitopes, hormones (e.g., glucocorticosteroids, opioid peptides, steroids, etc.), hormone receptors, peptides, enzymes, enzyme substrates, co-factors, lectins, sugars, oligonucleotides or nucleic acids, oligosaccharides, proteins, small molecules and monoclonal antibodies.

[0069] As used herein, the terms "cells," "host cells" or "recombinant host cells" are used interchangeably and mean not only to the particular subject cell, but also to the progeny or potential progeny of such a cell. Because certain modifications can occur in succeeding generations due to either mutation or environmental influences, such progeny might not, in fact, be identical to the parent cell, but are still included within the scope of the term as used herein.

[0070] As used herein, the terms "chimeric protein" or "fusion protein" are used interchangeably and mean a fusion of a first amino acid sequence encoding a target polypeptide with a second amino acid sequence defining a polypeptide domain foreign to, and not homologous with, any domain of a target polypeptide. A chimeric protein can include a foreign domain that is found in an organism that also expresses the first protein, or it can be an "interspecies" or "intergenic" fusion of protein structures expressed by different kinds of organisms. In general, a fusion protein can be represented by the general formula X--target--Y, wherein "target" represents a portion of the protein that is derived from a target polypeptide, and X and Y are independently absent or represent amino acid sequences that are not

related to a target sequence in an organism, including naturally occurring mutants. Representative target polypeptides include, but are not limited to, GR, AR, MR, PR and other NRs.

[0071] As used herein, the term "co-activator" means an entity that has the ability to enhance transcription when it is bound to at least one other entity. The association of a co-activator with an entity has the ultimate effect of enhancing the transcription of one or more sequences of DNA. In the context of the present invention, transcription is preferably nuclear receptor-mediated. By way of specific example, in the present invention TIF2 (the human analog of mouse glucocorticoid receptor interaction protein 1 (GRIP1)) can bind to a site on the glucocorticoid receptor, an event that can enhance transcription. TIF2 is therefore a co-activator of the glucocorticoid receptor. Other GR co-activators can include SRC1.

[0072] As used herein, the term "co-repressor" means an entity that has the ability to repress transcription when it is bound to at least one other entity. In the context of the present invention, transcription is preferably nuclear receptor-mediated. The association of a co-repressor with an entity has the ultimate effect of repressing the transcription of one or more sequences of DNA.

[0073] As used herein, the term "crystal lattice" means the array of points defined by the vertices of packed unit cells.

[0074] As used herein, the term "detecting" means confirming the presence of a target entity by observing the occurrence of a detectable signal, such as a radiologic or spectroscopic signal that will appear exclusively in the presence of the target entity.

[0075] As used herein, the term "DNA segment" means a DNA molecule that has been isolated free of total genomic DNA of a particular species. In a preferred embodiment, a DNA segment encoding a GR polypeptide refers to a DNA segment that comprises any of SEQ ID NOs: 1, 3, 5 and 7, but can optionally comprise fewer or additional nucleic acids, yet is isolated away from, or purified free from, total genomic DNA of a source species, such as *Homo sapiens*. Included within the term "DNA segment" are DNA segments and smaller fragments of such segments, and also recombinant vectors, including, for example, plasmids, cosmids, phages, viruses, and the like.

[0076] As used herein, the term "DNA sequence encoding a GR polypeptide" can refer to one or more coding sequences within a particular individual. Moreover, certain differences in nucleotide sequences can exist between individual organisms, which are called alleles. It is possible that such allelic differences might or might not result in differences in the amino acid sequence of the encoded polypeptide yet still encode a protein with the same biological activity. As is well known, genes for a particular polypeptide can exist in single or multiple copies within the genome of an individual. Such duplicate genes can be identical or can have certain modifications, including nucleotide substitutions, additions or deletions, all of which still code for polypeptides having substantially the same activity.

[0077] As used herein, the phrase "enhancer-promoter" means a composite unit that contains both enhancer and promoter elements. An enhancer-promoter is operatively linked to a coding sequence that encodes at least one gene product.

[0078] As used herein, the term "expanded binding pocket" means an NR ligand binding pocket in which atoms in the protein have shifted so as to increase the volume available to the ligand. The GR/FP structure disclosed in Table 2 provides an example in which, in the A-subunit, the pocket volume increases by approximately 58 cubic angstroms compared with the corresponding subunit of the GR/Dex structure, as described in Table 3, and in which, in the B-subunit, the pocket volume increases by approximately 138 cubic angstroms compared with the corresponding subunit of the GR/Dex structure. In this example, the expansion in the pocket volume is due to movements in atoms comprising residues M560, L563, M639, Q642, M646, and Y735.

[0079] Although a GR expanded binding pocket has been described, other NRs can also comprise an expanded binding pocket. For example, residues that are homologous to those listed for GR (i.e. M560, L563, M639, Q642, M646, and Y735) can be sterically displaced in other NRs. Figure 17, which depicts an alignment of several NRs, can be employed to identify residues homologous to those identified for GR. Figures 8A and 8B identify residues of GR subunit A and subunit B, respectively, that interact with an FP ligand. Steric displacement of any residue in an NR that is homologous to those identified in Figures 8A and 8B for a given NR can also contribute to an expanded binding pocket. Thus, an expanded binding pocket can be formed by steric displacement of one or more residues homologous to the GR residues identified in Figures 8A, 8B and 17.

[0080] An expanded binding pocket can also be characterized in terms of steric displacement of secondary structure elements. Referring again to GR, when FP is bound to the ligand binding site, helices 3, 6, 7, 10 and the loop preceding the AF-2 helix are sterically displaced, leading to an increase in pocket volume as compared with a GR/Dex structure, as characterized by the atomic coordinates of Table 3. Displacement of homologous secondary structure in other NRs can lead to an increase in the pocket volume. Figure 17 identifies homologous secondary structure for several nuclear receptors.

[0081] An expanded NR binding pocket comprises a greater volume than the ligand binding pocket volume in other structures of the same NR. The term "binding pocket volume," which refers to the volume of a binding pocket further defines the term "expanded binding pocket," can also be characterized by reference to the following Table of Pocket Volume Data, which tabulates some representative pocket volumes. In the Table of Pocket Volume Data, pocket vol-

umes were calculated with the program GRASP, using a grid spacing of 0.20 angstroms for construction of the molecular surface, with the atomic radius values of Bondi (Bondi, (1964) *J. Phys. Chem.* 68:441-451), and using a procedure in the MVP program to close all openings and channels connecting the pocket with the exterior of the protein. Ligand volumes were also calculated with the program GRASP, using the same grid spacing and atomic radius values. The specific radius values are as follows: hydrogen, 1.20 angstroms (Å); carbon, 1.70 Å; oxygen, 1.52 Å; nitrogen, 1.55 Å; sulfur, 1.80 Å; fluorine, 1.47 Å; chlorine, 1.75 Å; bromine, 1.85 Å; iodine, 1.98 Å. Hydrogen atoms are modeled onto the protein and the ligand using standard bond lengths and angles, and are represented explicitly in the volume calculations. The MVP program closes openings and channels by covering the entire protein with several layers of closely spaced spheres of radius 1.4 angstroms, and then classifying the spheres as either "inside" or "outside" the protein, based on the degree to which the protein buries the spheres. For the pocket volume calculations, the spheres classified as "outside" are loaded into GRASP together with the protein atoms. This procedure effectively closes all the openings and channels that connect the pocket to the outside of the protein, and allows GRASP to calculate a meaningful cavity volume for the pocket. In the following Table of Pocket Volume Data, all volumes are given in cubic angstroms.

Table of Pocket Volume Data					
protein	ligand	subunit-A		subunit-B	
		pocket	ligand	pocket	ligand
GR	fluticasone proionate	658	476	716	477
GR	dexamethasone	600	390	578	389
PR	progesterone	557	349	570	351
AR	dihydrotestosterone	422	319	no B subunit	

[0082] The term "expanded binding pocket," then, can refer to an NR ligand binding pocket in which the pocket volume is increased by about 50 cubic angstroms over that of a ligand binding pocket in a different structure of the same NR. By way of example, a GR LBD of the present invention comprising an expanded binding pocket (e.g. as characterized by the atomic structural coordinates of Table 2) can exhibit an increase in pocket volume of between about 50 and about 150 cubic angstroms over a GR structure lacking an expanded binding pocket, (e.g. as characterized by the atomic coordinates of Table 3). In other examples, an AR LBD comprising an expanded binding pocket (e.g. as characterized by the atomic structural coordinates of Table 4) can exhibit an increase in pocket volume of between about 50 and about 150 cubic angstroms over an AR structure lacking an expanded binding pocket (e.g. as characterized by the atomic structural coordinates of Tables 8 and 9). A MR LBD comprising an expanded binding pocket (e.g. as characterized by the atomic structural coordinates of Table 11) can exhibit an increase in pocket volume of between about 50 and about 150 cubic angstroms over a MR structure lacking an expanded binding pocket. A PR LBD comprising an expanded binding pocket (e.g. as characterized by the atomic structural coordinates of Table 5) can exhibit an increase in pocket volume of between about 50 and about 150 cubic angstroms over a PR structure lacking an expanded binding pocket (e.g. as characterized by the atomic structural coordinates of Table 10).

[0083] In a preferred embodiment, a GR structure with an expanded binding pocket can comprise a crystalline GR polypeptide, with or without ligand, and with or without coactivator peptide, and atomic coordinates thereof, where the AF2 helix is located in the active position, and where atoms in the residues Met560, Met639, Gln642, Cys643, Met646, and Tyr735 have shifted from their positions in a GR/Dex structure, e.g. as characterized by the atomic structural coordinates of Table 3, by a heavy-atom RMS deviation of at least about 0.50 angstroms, or by a backbone heavy-atom RMS deviation of at least about 0.35 angstroms.

[0084] In another preferred embodiment, a GR structure with an expanded binding pocket can comprise a crystalline GR polypeptide, with or without ligand, and with or without coactivator peptide, and atomic coordinates thereof, where the AF2 helix is located in the active position, and where atoms in the residues Met560, Met639, Gln642, Cys643, Met646, and Tyr735 have shifted from their positions in a GR/Dex structure, e.g. as characterized by the atomic structural coordinates of Table 3, so as to increase the volume of a binding pocket by at least about 5% compared with a GR/Dex structure, e.g. as characterized by the atomic structural coordinates of Table 3.

[0085] In yet another preferred embodiment, a GR structure with an expanded binding pocket can comprise a crystalline GR polypeptide, with or without ligand, and with or without coactivator peptide, and atomic coordinates thereof, where the AF2 helix is located in the active position, and where atoms in and around the ligand binding site have shifted from their positions in the GR/Dex structure so as to accomodate without atomic overlap steroidal ligands with C17- α substituents comprising 2-20 heavy atoms.

[0086] In a further preferred embodiment, a GR structure with an expanded binding pocket can comprise a crystalline GR polypeptide, with or without ligand, and with or without coactivator peptide, and atomic coordinates thereof, where

the AF2 helix is located in the active position, and where atoms in and around the ligand binding site have shifted from their positions in the GR/Dex structure so as to accomodate without atomic overlap non-steroidal ligands such as benzoxazin-1-one and A-222977.

[0087] In an additional preferred embodiment, a GR structure with an expanded binding pocket can comprise a crystalline GR polypeptide, with or without ligand, and with or without coactivator peptide, and atomic coordinates thereof, where the AF2 helix is located in the active position, and where atoms in and around the ligand binding site have shifted from their positions in the GR/Dex structure so that fluticasone propionate can be docked into the binding site with a favorable binding energy, as computed with molecular modeling software such as MVP, Discover, AMBER or CHARMM, using common force fields such as CFF91 or MMFF94, and where all atoms in the protein are held fixed.

[0088] In another preferred embodiment, a GR structure with an expanded binding pocket can comprise a crystalline GR polypeptide, with or without ligand, and with or without coactivator peptide, and atomic coordinates thereof, where the AF2 helix is located in the active position, and where atoms in and around the ligand binding site have shifted from their positions in the GR/Dex structure so that non-steroidal GR ligands, such as benzoxazin-1-one and A-222977, can be docked into the binding site with a favorable binding energy, as computed with molecular modeling software such as MVP, Discover, AMBER or CHARMM, using common force fields such as CFF91 or MMFF94, and where all atoms in the protein are held fixed.

[0089] As used herein, the term "expression" generally refers to the cellular processes by which a biologically active polypeptide is produced.

[0090] As used herein, the term "gene" is used for simplicity to refer to a functional protein, polypeptide or peptide encoding unit. As will be understood by those in the art, this functional term includes both genomic sequences and cDNA sequences. Preferred embodiments of genomic and cDNA sequences are disclosed herein.

[0091] As used herein, the term "glucocorticoid" means a steroid hormone glucocorticoid. "Glucocorticoids" are agonists for the glucocorticoid receptor. Compounds which mimic glucocorticoids can also be defined as glucocorticoid receptor agonists. A preferred glucocorticoid receptor agonist is fluticasone propionate. Other common glucocorticoid receptor agonists include cortisol, cortisone, prednisolone, prednisone, methylprednisolone, triamcinolone, hydrocortisone, and corticosterone. As used herein, glucocorticoid is intended to include, for example, the following generic and brand name corticosteroids: cortisone (CORTONE ACETATE, ADRESON, ALTESONA, CORTELAN, CORTISTAB, CORTISYL, CORTOGEN, CORTONE, SCHEROSON); dexamethasone--oral (DECADRON-ORAL, DEXAMETH, DEXONE, HEXADROL-ORAL, DEXAMETHASONE INTENSOL, DEXONE 0.5, DEXONE 0.75, DEXONE 1.5, DEXONE 4); hydrocortisone--oral (CORTEF, HYDROCORTONE); hydrocortisone cypionate (CORTEF ORAL SUSPENSION); methylprednisolone--oral (MEDROL-ORAL); prednisolone--oral (PRELONE, DELTA-CORTEF, PEDIAPRED, ADNISOLONE, CORTALONE, DELTACORTRIL, DELTASOLONE, DELTASTAB, DI-ADRESON F, ENCORTOLONE, HYDROCORTANCYL, MEDISOLONE, METICORTELONE, OPREDSONE, PANAAFECORTELONE, PRECORTISYL, PRENISOLONA, SCHERISOLONA, SCHERISOLONE); prednisone (DELTASONE, LIQUID PRED, METICORTEN, ORASONE 1, ORASONE 5, ORASONE 10, ORASONE 20, ORASONE 50, PREDNICEN-M, PREDNISONE INTENSOL, STERAPRED, STERAPRED DS, ADASONE, CARTANCYL, COLISONE, CORDROL, CORTAN, DACORTIN, DECORTIN, DECORTISYL, DELCORTIN, DELLACORT, DELTA-DOME, DELTACORTENE, DELTISONA, DI-ADRESON, ECONOSONE, ENCORTON, FERNISONE, NISONA, NOVOPREDNISONE, PANAFECORT, PANASOL, PARACORT, PARMENISON, PEHACORT, PREDELTIN, PREDNICORT, PREDNICOT, PREDNIDIB, PREDNIMENT, RECTODELT, ULTRACORTEN, WINPRED); triamcinolone--oral (KENACORT, ARISTOCORT, ATOLONE, SHOLOG A, TRAMACORT-D, TRI-MED, TRIAMCOT, TRISTO-PLEX, TRYLONE D, U-TRI-LONE).

[0092] As used herein, the term "glucocorticoid receptor," abbreviated herein as "GR," means the receptor for a steroid hormone glucocorticoid. A glucocorticoid receptor is a steroid receptor and, consequently, a nuclear receptor, since steroid receptors are a subfamily of the superfamily of nuclear receptors. The term "GR" means any polypeptide sequence that can be aligned with human GR such that at least 70%, preferably at least 75%, of the amino acids are identical to the corresponding amino acid in the human GR. The term "GR" also encompasses nucleic acid sequences where the corresponding translated protein sequence can be considered to be a GR. The term "GR" includes invertebrate homologs, whether now known or hereafter identified; preferably, GR nucleic acids and polypeptides are isolated from eukaryotic sources. The term "GR" further includes vertebrate homologs of GR family members, including, but not limited to, mammalian and avian homologs. Representative mammalian homologs of GR family members include, but are not limited to, murine and human homologs. The term "GR" specifically encompasses all GR isoforms, including GR α and GR β . GR β is a splicing variant with 100% identity to GR α , except at the C-terminus, where 50 residues in GR α have been replaced with 15 residues in GR β .

[0093] As used herein, the terms "GR gene product", "GR protein", "GR polypeptide", and "GR peptide" are used interchangeably and mean peptides having amino acid sequences which are substantially identical to native amino acid sequences from the organism of interest and which are biologically active in that they comprise all or a part of the amino acid sequence of a GR polypeptide, or cross-react with antibodies raised against a GR polypeptide, or retain all or some of the biological activity (e.g., DNA or ligand binding ability and/or transcriptional regulation) of the native

amino acid sequence or protein. Such biological activity can include immunogenicity. Representative embodiments are set forth in SEQ ID NOs: 2, 4, 6, and 8. The terms "GR gene product", "GR protein", "GR polypeptide", and "GR peptide" also include analogs of a GR polypeptide. By "analog" is intended that a DNA or peptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some of the biological activity of those sequences.

5 Analogs can be derived from genomic nucleotide sequences as are disclosed herein or from other organisms, or can be created synthetically. Those skilled in the art will appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct GR analogs. There is no need for a "GR gene product", "GR protein", "GR polypeptide", or "GR peptide" to comprise all or substantially all of the amino acid sequence of a GR polypeptide gene product. Shorter or longer sequences are anticipated to be of use in the invention; shorter sequences are herein referred to as "segments". Thus, the terms "GR gene product", "GR protein", "GR polypeptide", and "GR peptide" also include fusion or recombinant GR polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein and are known in the art.

10 [0094] As used herein, the terms "GR gene" and "recombinant GR gene" mean a nucleic acid molecule comprising an open reading frame encoding a GR polypeptide of the present invention, including both exon and (optionally) intron sequences.

15 [0095] As used herein, "hexagonal unit cell" means a unit cell wherein $a = b \neq c$; and $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$. The vectors a , b and c describe the unit cell edges and the angles α , β , and γ describe the unit cell angles. In a preferred embodiment of the present invention, the unit cell has lattice constants of $a = b = 127.656 \text{ \AA}$, $c = 87.725 \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 120^\circ$. While preferred lattice constants are provided, a crystalline polypeptide of the present invention also comprises variations from the preferred lattice constants, wherein the variations range from about one to about two percent. Thus, for example, a crystalline polypeptide of the present invention can also comprise lattice constants a and b of about 126 \AA or about 128 \AA and lattice constant c of about 86 \AA or about 88 \AA .

20 [0096] As used herein, "homology model" or "homology modeling" means a simulated three-dimensional protein structure resulting from homology modeling, which encompasses the process of creating those simulated protein structures by systematic replacement of differing amino acid residues in a related template protein structure, that can either be a crystal structure or homology model itself, in order to produce a target protein structure.

25 [0097] As used herein, "docking model" means a simulated three-dimensional protein structure resulting from the manual or automated adjustment of the three-dimensional coordinates of a template protein structure, that can either be a crystal structure or homology model, and/or a bound ligand. A docking model differs from a homology model in that, when constructing a docking model, no systematic replacement of differing amino acids residues is required.

30 [0098] As used herein, "model" means either a homology model or a docking model depending on the context.

[0099] As used herein, the term "hybridization" means the binding of a probe molecule, e.g. a molecule to which a detectable moiety has been bound, to a target sample.

35 [0100] As used herein, the term "interact" means detectable interactions between molecules, such as can be detected using, for example, a yeast two hybrid assay. The term "interact" is also meant to include "binding" interactions between molecules. Interactions can, for example, be protein-protein or protein-nucleic acid in nature.

[0101] As used herein, the term "intron" means a DNA sequence present in a given gene that is not translated into protein.

40 [0102] As used herein, the term "isolated" means oligonucleotides substantially free of other nucleic acids, proteins, lipids, carbohydrates or other materials with which they can be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to polypeptides, in which case the polypeptide will be substantially free of nucleic acids, carbohydrates, lipids and other undesired polypeptides.

[0103] As used herein, the term "labeled" means the attachment of a moiety, capable of detection by spectroscopic, radiologic or other methods, to a probe molecule.

45 [0104] As used herein, the term "modified" means an alteration from an entity's normally occurring state. An entity can be modified by removing discrete chemical units or by adding discrete chemical units. The term "modified" encompasses detectable labels as well as those entities added as aids in purification.

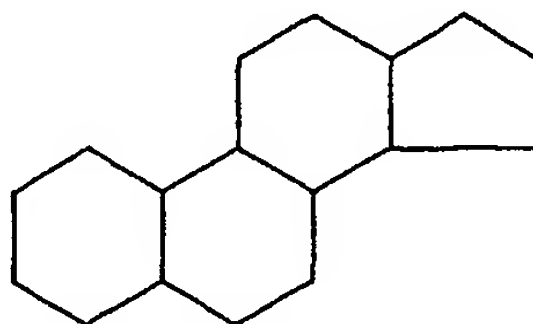
50 [0105] As used herein, the term "modulate" means an increase, decrease, or other alteration of any or all chemical and biological activities or properties of a wild-type or mutant polypeptide, e.g. a wild-type or mutant GR polypeptide. The term "modulation" as used herein refers to both upregulation (i.e., activation or stimulation) and downregulation (i.e. inhibition or suppression) of a response, and includes responses that are upregulated in one cell type or tissue, and down-regulated in another cell type or tissue.

55 [0106] As used herein, the term "molecular replacement" means a method of solving a crystal structure of a chemical compound (e.g. a protein) that involves generating a preliminary model of a crystalline polypeptide whose structure coordinates are unknown (e.g. a wild type or mutant GR polypeptide or fragment or domain thereof), by orienting and positioning a molecule or model whose structure coordinates are known (e.g., a nuclear receptor) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis

of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. See, e.g., Lattman, (1985) *Method Enzymol.*, 115: 55-77; Rossmann (ed.), (1972) *The Molecular Replacement Method*, Gordon & Breach, New York, New York, United States of America. For example, using the structure coordinates of the ligand binding domain of GR provided by this invention,

[0107] As used herein, the term "mutation" carries its traditional connotation and means a change, inherited, naturally occurring or introduced, in a nucleic acid or polypeptide sequence, and is used in its sense as generally known to those of skill in the art.

[0108] As used herein, the terms "non-steroid" and "non-steroid compound" are used interchangeably and mean a compound that lacks the ring structure that defines steroid compounds, namely the structure:



but retains the binding and functional activity of a steroid compound for an NR such as GR.

[0109] As used herein, the term "nuclear receptor", occasionally abbreviated herein as "NR", means a member of the superfamily of receptors that comprises at least the subfamilies of steroid receptors, thyroid hormone receptors, retinoic acid receptors and vitamin D receptors, and specifically encompasses GR. Thus, a given nuclear receptor can be further classified as a member of a subfamily while retaining its status as a nuclear receptor. The term "nuclear receptor" also encompasses fragments of a nuclear receptor.

[0110] As used herein, the phrase "operatively linked" means that an enhancer-promoter is connected to a coding sequence in such a way that the transcription of that coding sequence is controlled and regulated by that enhancer-promoter. Techniques for operatively linking an enhancer-promoter to a coding sequence are well known in the art; the precise orientation and location relative to a coding sequence of interest is dependent, *inter alia*, upon the specific nature of the enhancer-promoter.

[0111] As used herein, the term "partial agonist" means an entity that can bind to a receptor or other target and induce only part of the changes in the receptor or other target that are induced by agonists. The differences can be qualitative or quantitative. Thus, a partial agonist can induce some of the conformation changes induced by agonists, but not others, or it can only induce certain changes to a limited extent.

[0112] As used herein, the term "partial antagonist" means an entity that can bind to a receptor or other target and inhibit only part of the changes in the receptor or other target that are induced by antagonists. The differences can be qualitative or quantitative. Thus, a partial antagonist can inhibit some of the conformation changes induced by an antagonist, but not others, or it can inhibit certain changes to a limited extent.

[0113] As used herein, the term "pocket volume" means the volume of space within the protein that is available for occupation by a ligand. Any desired algorithm can be employed when calculating a pocket volume, although some algorithms are more accurate than others. In one approach, a pocket volume can be approximated by an ellipsoid with principle axes of length 2a, 2b and 2c, and its volume can be calculated as

$$V = (4/3) \times \pi \times (a) \times (b) \times (c)$$

where $\pi=3.14159$.

[0114] The walls of the pocket are formed from atoms comprising the nuclear receptor protein. In another approach, these atoms, and the atoms in the ligand, can be approximated as spheres with specified atomic radius values. With this representation, the walls of the pocket comprise numerous spheres. If two atoms are directly bonded together, then their spheres will overlap. The spheres can also overlap when atoms are connected together by bonds with one or two intervening atoms, but do not normally overlap significantly when atoms are more distantly connected, or when the atoms are not covalently connected. Consequently, in this representation, the walls of the pocket have numerous gaps, channels and spaces between the spheres. Ligand atoms may fit into some of the larger gaps, channels and spaces, but generally cannot fit into the smaller gaps, channels and spaces. This complication of the spherical atom representation led to the definition of a "molecular surface" where gaps and spaces too small to accommodate a water

molecule, or "probe," were effectively smoothed over. Some of the fundamental issues involved in the definition of a molecular surface and the calculation of molecular volumes are discussed in Richards, (1977) Ann. Rev. Biophys. Bioeng. 6:151-176. For a further discussion of the molecular surface and algorithms for its calculation, see Connolly, (1983) *Science* 221:709-713. Because of Connolly's contributions, the molecular surface is sometimes referred to as a "Connolly surface."

[0115] A pocket is generally defined as the region enclosed by the molecular surface, where the molecular surface is calculated using a probe radius of 1.4 angstroms. With nuclear receptors, there can often be channels connecting the pocket with the exterior of the protein. In this case, it is presumed that the channels are occluded in some manner so that a fully enclosed pocket can be defined. For example, a channel can be occluded by placing a water molecule at the narrowest point along the channel. The program MVP has a systematic algorithm for closing channels: the entire protein is first covered by several layers of closely-spaced water-sized spheres. The spheres are generated by placing the protein in a grid, and identifying grid points where a sphere of radius 1.4 angstroms can be accommodated without overlapping the sphere corresponding to any atom of the protein. In calculations reported herein, the grid spacing was taken as 0.3-0.8 angstroms. These spheres on the grid are then identified as either internal to the protein or external to the protein, based on the degree to which they are buried within the protein. The degree of burial is quantified by measuring the solid angle occluded by the protein at the grid point in question. In calculations reported herein, the sphere is considered to be buried if 90% or more of the solid angle is occluded by the protein.

[0116] A fully closed molecular surface can be generated for the ligand binding pocket with programs such as GRASP (Columbia University, New York, New York, United States of America) or Connolly's MS program by loading the protein together with the external water-sized spheres generated by MVP. The program GRASP can further be used to calculate the cavity volume. It is noted that the calculated cavity volume is sensitive to the grid spacing used in generating the molecular surface. The GRASP calculations reported herein used a grid spacing of 0.2 angstroms. Coarser spacings can lead to substantially inaccurate volumes. The internal grid spheres generated by MVP can also be used to estimate the volume of the pocket. In this case, MVP carries out a cluster analysis to group the internal spheres into clusters corresponding to different pockets and cavities within the protein. With nuclear receptors, the ligand binding pocket generally corresponds to the largest such cluster. The volume of the cluster can be calculated directly with the GRASP program. This approach tends to underestimate the volume of the pocket, since the internal grid spheres can never fill the pocket entirely. The spheres can fill the pocket more fully as the grid spacing is reduced. A grid spacing of 0.3 angstroms gives volumes in relatively good agreement with the alternative GRASP method described above. Other methods of calculating pocket volumes have been described in the literature. See, e.g., Kleywegt & Jones, (1994) Acta Crystallogr. Section D 50:178-185.

[0117] Aside from the algorithm used, the atomic radius values can also be considered. Generally, atomic volumes depend on the radius raised to the third power, so it is clear that calculated molecular volumes are sensitive to atomic radius values. Cavity volumes tend to decrease as radius values increase, and if the atomic radius values are too large, the calculated cavity volume will be too small. In the present invention, the following atomic radius values were employed: hydrogen, 1.20Å; carbon, 1.70Å; nitrogen, 1.55Å; oxygen, 1.52Å; sulfur, 1.80Å; fluorine, 1.47Å; chlorine, 1.75Å; bromine, 1.85Å; iodine, 1.98Å. See Bondi, (1964) J. Phys. Chem. 68:441-451. For all volume calculations reported herein, the hydrogens were represented explicitly. These hydrogen atoms are added to the protein with MVP using standard bond lengths and angles, followed by energy minimization with the CFF91 force field within MVP. Some other workers in the protein structure field often omit the hydrogens in surface and volume calculations, using an increased carbon radius to compensate. This "united atom" approximation can reduce the accuracy of a pocket volume calculation.

[0118] When comparing the volumes of two different proteins, or two different conformations of the same protein, it is preferable to use the same algorithm, parameters and atomic radius values.

[0119] As used herein, the term "polypeptide" means any polymer comprising any of the 20 protein amino acids, regardless of its size. Although "protein" is often used in reference to relatively large polypeptides, and "peptide" is often used in reference to small polypeptides, usage of these terms in the art overlaps and varies. The term "polypeptide" as used herein refers to peptides, polypeptides and proteins, unless otherwise noted. As used herein, the terms "protein", "polypeptide" and "peptide" are used interchangeably herein when referring to a gene product.

[0120] As used herein, the term "primer" means a sequence comprising two or more deoxyribonucleotides or ribonucleotides, preferably more than three, and more preferably more than eight and most preferably at least about 20 nucleotides of an exonic or intronic region. Such oligonucleotides are preferably between ten and thirty bases in length.

[0121] As used herein, the term "root mean squared (RMS) deviation" of a collection of atoms in one protein structure relative to the corresponding atoms in another protein structure refers to the average displacement of those atoms, after superimposition of the proteins, as computed according to the formula

$$\text{RMSDeviation} = \sqrt{\frac{1}{N} \sum_{i=1}^N \left[(x_i^1 - x_i^2)^2 + (y_i^1 - y_i^2)^2 + (z_i^1 - z_i^2)^2 \right]}$$

5

where x_i^1 , y_i^1 , z_i^1 are the coordinates of atom i in structure 1, and x_i^2 , y_i^2 , z_i^2 are the coordinates of atom i in structure 2 (after superimposition of the two proteins), N is the number of atoms in the collection, and where the index i runs iteratively through the collection of N atoms for which the RMS deviation is to be calculated. The superimposition is a rotation and translation of the coordinates carried out using the backbone atoms in the core of the protein, and carried out so as to minimize the RMS deviation of these core backbone atoms. This can optionally include some or all the atoms in the collection for which the RMS deviation is calculated. For GR, the superimposition might be carried out using backbone atoms in helices 1-10, but would normally not include the AF2 helix or the loops connecting the helices. Various algorithms are available for generating the rotation matrix and translation vectors that superimpose two sets of protein backbone atoms. See, for example, Kabsch, (1978) *Acta Cryst.* A34, 827-828. These algorithms can be used together with sequence alignment algorithms to identify corresponding backbone atoms in two different protein structures. See, for example, Blundell et al., (1987) *Nature* 326:347-352. Hydrogen atoms are generally not clearly visible in the electron density, and there may be uncertainties in their placement using molecular modeling software. Consequently, hydrogen atoms are usually not included in the collections of atoms used in calculating RMS deviations. As used herein, the term heavy atom RMS deviation refers to an RMS deviation calculated by excluding the hydrogen atoms from the specified collection. In the analysis of protein structures, the side-chain atoms often shift more than the backbone atoms, and it may be useful to calculate RMS deviations using only the backbone heavy atoms. As used herein, the term backbone heavy-atom RMS deviation refers to an RMS deviation calculated using the backbone heavy atoms, commonly designated as N, C α , C and O, but not including any of the side-chain atoms.

[0122] As used herein, the term "sequencing" means the determining the ordered linear sequence of nucleic acids or amino acids of a DNA or protein target sample, using conventional manual or automated laboratory techniques.

[0123] As used herein, the term "space group" means the arrangement of symmetry elements of a crystal.

[0124] As used herein, the term "steroid receptor" means a nuclear receptor that can bind or associate with a naturally occurring steroid compound. Steroid receptors are a subfamily of the superfamily of nuclear receptors. The subfamily of steroid receptors comprises glucocorticoid receptors and, therefore, a glucocorticoid receptor is a member of the subfamily of steroid receptors and the superfamily of nuclear receptors.

[0125] As used herein, the terms "structure coordinates," "structural coordinates," "spatial coordinates," "atomic structure coordinates," "three-dimensional coordinates" and "atomic coordinates" are used interchangeably and mean mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

[0126] Those of skill in the art understand that a set of coordinates determined by X-ray crystallography is not without standard error. In general, the error in the coordinates tends to be reduced as the resolution is increased, since more experimental diffraction data is available for the model fitting and refinement. Thus, for example, more diffraction data can be collected from a crystal that diffracts to a resolution of 3.0 angstroms than from a crystal that diffracts to a lower resolution, such as 3.5 angstroms. Consequently, the refined structural coordinates will usually be more accurate when fitted and refined using data from a crystal that diffracts to higher resolution. The design of ligands and modulators for GR or any other NR depends on the accuracy of the structural coordinates. If the coordinates are not sufficiently accurate, then the design process will be ineffective. In most cases, it is very difficult or impossible to collect sufficient diffraction data to define atomic coordinates precisely when the crystals diffract to a resolution of only 3.5 angstroms or poorer. Thus, in most cases, it is difficult to use X-ray structures in structure-based ligand design when the X-ray structures are based on crystals that diffract to a resolution of only 3.5 angstroms or poorer. However, common experience has shown that crystals diffracting to 3.0 angstroms or better can yield X-ray structures with sufficient accuracy to greatly facilitate structure-based drug design. Further improvement in the resolution can further facilitate structure-based design, but the coordinates obtained at 3.0 angstroms resolution are generally adequate for most purposes.

[0127] Also, those of skill in the art will understand that NR proteins can adopt different conformations when different ligands are bound. In particular, NR proteins will adopt substantially different conformations when agonists and antagonists are bound. Subtle variations in the conformation can also occur when different agonists are bound, and when different antagonists are bound. These variations can be difficult or impossible to predict from a single X-ray structure. Generally, structure-based design of GR modulators depends to some degree on an understanding of the differences in conformation that occur when agonists and antagonists are bound. Thus, structure-based modulator design is most facilitated by the availability of X-ray structures of complexes with potent agonists as well as potent antagonists.

[0128] As used herein, the term "substantially pure" means that the polynucleotide or polypeptide is substantially free of the sequences and molecules with which it is associated in its natural state, and those molecules used in the isolation procedure. The term "substantially free" means that the sample is at least 50%, preferably at least 70%, more preferably 80% and most preferably 90% free of the materials and compounds with which it is associated in nature.

[0129] As used herein, the term "target cell" refers to a cell, into which it is desired to insert a nucleic acid sequence or polypeptide, or to otherwise effect a modification from conditions known to be standard in the unmodified cell. A nucleic acid sequence introduced into a target cell can be of variable length. Additionally, a nucleic acid sequence can enter a target cell as a component of a plasmid or other vector or as a naked sequence.

[0130] As used herein, the term "transcription" means a cellular process involving the interaction of an RNA polymerase with a gene that directs the expression as RNA of the structural information present in the coding sequences of the gene. The process includes, but is not limited to the following steps: (a) the transcription initiation, (b) transcript elongation, (c) transcript splicing, (d) transcript capping, (e) transcript termination, (f) transcript polyadenylation, (g) nuclear export of the transcript, (h) transcript editing, and (i) stabilizing the transcript.

[0131] As used herein, the term "transcription factor" means a cytoplasmic or nuclear protein which binds to such gene, or binds to an RNA transcript of such gene, or binds to another protein which binds to such gene or such RNA transcript or another protein which in turn binds to such gene or such RNA transcript, so as to thereby modulate expression of the gene. Such modulation can additionally be achieved by other mechanisms; the essence of "transcription factor for a gene" is that the level of transcription of the gene is altered in some way.

[0132] As used herein, the term "unit cell" means a basic parallelepiped shaped block. The entire volume of a crystal can be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal. Thus, the term "unit cell" means the fundamental portion of a crystal structure that is repeated infinitely by translation in three dimensions. A unit cell is characterized by three vectors a, b, and c, not located in one plane, which form the edges of a parallelepiped. Angles α , β and γ define the angles between the vectors: angle α is the angle between vectors b and c; angle β is the angle between vectors a and c; and angle γ is the angle between vectors a and b. The entire volume of a crystal can be constructed by regular assembly of unit cells; each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

II. Description of Tables

[0133] Table 1 is a table summarizing the crystal and data statistics obtained from the crystallized ligand binding domain of human GR in complex with the ligand fluticasone propionate and a coactivator peptide derived from TIF2. Data on the unit cell are presented, including data on the crystal space group, unit cell dimensions, molecules per asymmetric cell and crystal resolution.

[0134] Table 2 is a table presenting the atomic coordinate data for crystallized GR LBD in complex with fluticasone propionate and a TIF2 peptide.

[0135] Table 3 is a table presenting the atomic coordinate data for human GR in complex with dexamethasone and a TIF2 peptide employed in the molecular replacement solution of human GR ligand binding domain in complex with fluticasone propionate and a TIF2 peptide.

[0136] Table 4 is a table presenting the three-dimensional coordinates of AR in complex with bicalutamide obtained from homology modeling of the crystal structure coordinates of GR α in complex with FP.

[0137] Table 5 is a table presenting the three-dimensional coordinates of PR in complex with RWJ-60130 obtained from homology modeling of the crystal structure coordinates of GR α in complex with FP.

[0138] Table 6 is a table presenting a subset of three-dimensional coordinates of GR α in complex with the benzoxazin-1-one obtained from modeling of the crystal structure of GR α in complex with FP.

[0139] Table 7 is a table presenting a subset of three-dimensional coordinates of GR α in complex with A-222977 obtained from modeling of the crystal structure of GR α in complex with FP.

[0140] Table 8 is a table presenting three-dimensional coordinates of AR in complex with DHT (Sack et al., (2001) *Proc. Natl. Acad. Sci. U.S.A.* 98(9): 4904-4909; PDB ID No. 1I37).

[0141] Table 9 is a table presenting three-dimensional coordinates of AR in complex with the ligand R1881 (Matias et al., (2000) *J. Biol. Chem.* 275(34): 26164-171; PDB ID No. 1E3G).

[0142] Table 10 is a table presenting three-dimensional coordinates of PR in complex with PG (Williams & Sigler, (1998) *Nature* 393:392-396; PDB ID No. 1A28).

[0143] Table 11 is a table presenting three-dimensional coordinates of MR obtained from homology modeling of the crystal structure coordinates of GR α in complex with FP.

III. General Considerations

[0144] The present invention will usually be applicable *mutatis mutandis* to nuclear receptors in general, more particularly to steroid receptors including MR, AR, PR, GR and isoforms thereof, and even more particularly to glucocorticoid receptors, as discussed herein, based, in part, on the patterns of nuclear receptor and steroid receptor structure and modulation. Some of these patterns have emerged as a consequence of the present disclosure, which in part discloses determining the three dimensional structure of the ligand binding domain of GR α having an expanded binding pocket in complex with fluticasone propionate and a fragment of the co-activator TIF2.

[0145] The nuclear receptor superfamily can be subdivided into two subfamilies: the GR subfamily (also referred to as the steroid receptors and denoted SRs), comprising GR, AR (androgen receptor), MR (mineralocorticoid receptor) and PR (progesterone receptor) and the thyroid hormone receptor (TR) subfamily, comprising TR, vitamin D receptor (VDR), retinoic acid receptor (RAR), retinoid X receptor (RXR), and most orphan receptors. This division has been made on the basis of DNA binding domain structures, interactions with heat shock proteins (HSP), and ability to form dimers.

[0146] Steroid receptors (SRs) form a subset of the superfamily of nuclear receptors. The glucocorticoid receptor is a steroid receptor and thus a member of the superfamily of nuclear receptors and the subset of steroid receptors. The human glucocorticoid receptor exists in two isoforms: GR α , which comprises 777 amino acids and GR β , which comprises 742 amino acids. As noted, the alpha isoform of human glucocorticoid receptor comprises 777 amino acids and is predominantly cytoplasmic in its unactivated, non-DNA binding form. When activated, it translocates to the nucleus. In order to understand the role played by the glucocorticoid receptor in the different cell processes, the receptor was mapped by transfecting receptor-negative and glucocorticoid-resistant cells with different steroid receptor constructs and reporter genes like chloramphenicol acyltransferase (CAT) or luciferase which had been covalently linked to a glucocorticoid responsive element (GRE). From these and other studies, four major functional domains have become evident.

[0147] From the amino terminal end to the carboxyl terminal end, these functional domains include the tau 1, DNA binding, and ligand binding domains in succession. The tau 1 domain spans amino acid positions 77-262 and regulates gene activation. The DNA binding domain is from amino acid positions 421-486 and has nine cysteine residues, eight of which are organized in the form of two zinc fingers analogous to *Xenopus* transcription factor IIIA. The DNA binding domain binds to the regulatory sequences of certain genes that are induced or deinduced by glucocorticoids. Amino acids 521 to 777 form the ligand binding domain, which binds glucocorticoid to activate the receptor. This region of the receptor also comprises a nuclear localization signal. Deletion of this carboxyl terminal end results in a receptor that is constitutively active for gene induction (up to 30% of wild type activity) and even more active for cell kill (up to 150% of wild type activity) (Giguere et al., (1986) *Cell* 46: 645-652; Hollenberg et al., (1987) *Cell* 49: 39-46; Hollenberg & Evans, (1988) *Cell* 55: 899-906; Hollenberg et al., (1989) *Cancer Res.* 49: 2292s-2294s; Oro et al., (1988) *Cell* 55: 1109-1114; Evans, (1989) in *Recent Progress in Hormone Research* (Clark, ed.) Vol. 45, pp. 1-27, Academic Press, San Diego, California, United States of America; Green & Chambon, (1987) *Nature* 325: 75-78; Picard & Yamamoto, (1987) *EMBO J.* 6: 3333-3340; Picard et al., (1990) *Cell Regul.* 1: 291-299; Godowski et al., (1987) *Nature* 325: 365-368; Miesfeld et al., (1987) *Science* 236:423-427; Danielsen et al., (1989) *Cancer Res.* 49: 2286s-2291s; Danielsen et al., (1987) *Molec. Endocrinol.* 1: 816-822; Umesono & Evans, (1989) *Cell* 57: 1139-1146.). Despite the aforementioned indirect characterization of the structure of GR α , until the present disclosure, a detailed three-dimensional model of the ligand binding domain of GR α in complex with fluticasone propionate has not been achieved.

[0148] GR subgroup members are tightly bound by heat shock protein(s) (HSP) in the absence of ligand, dimerize following ligand binding and dissociation of HSP, and show homology in the DNA half sites to which they bind. These half sites also tend to be arranged as palindromes. TR subgroup members tend to be bound to DNA or other chromatin molecules when unliganded, can bind to DNA as monomers and dimers, but tend to form heterodimers, and bind DNA elements with a variety of orientations and spacings of the half sites, and also show homology with respect to the nucleotide sequences of the half sites. ER does not belong to either subfamily, since it resembles the GR subfamily in hsp interactions, and the TR subfamily in nuclear localization and DNA-binding properties.

[0149] Most members of the superfamily, including orphan receptors, possess at least two transcription activation subdomains, one of which is constitutive and resides in the amino terminal domain (AF-1), and the other of which (AF-2) resides in the ligand binding domain, whose activity is regulated by binding of an agonist ligand. The function of AF-2 requires an activation domain (also called transactivation domain) that is highly conserved among the receptor superfamily. Most LBDs contain an activation domain. Some mutations in this domain abolish AF-2 function, but leave ligand binding and other functions unaffected. Ligand binding allows the activation domain to serve as an interaction site for essential co-activator proteins that function to stimulate (or in some cases, inhibit) transcription.

[0150] Analysis and alignment of amino acid sequences, and X-ray and NMR structure determinations, have shown that nuclear receptors have a modular architecture with three main domains:

- 1) a variable amino-terminal domain;
- 2) a highly conserved DNA-binding domain (DBD); and
- 3) a less conserved carboxy-terminal ligand binding domain (LBD).

In addition, nuclear receptors can have linker segments of variable length between these major domains.

[0151] Sequence analysis and X-ray crystallography, including the disclosure of the present invention have confirmed that GR also has the same general modular architecture, with the same three domains. The function of GR in human cells presumably requires all three domains in a single amino acid sequence. However, the modularity of GR permits different domains of each protein to separately accomplish certain functions. Some of the functions of a domain within the full-length receptor are preserved when that particular domain is isolated from the remainder of the protein. Using conventional protein chemistry techniques, a modular domain can sometimes be separated from the parent protein. Using conventional molecular biology techniques, each domain can usually be separately expressed with its original function intact or, as discussed herein below, chimeras comprising two different proteins can be constructed, wherein the chimeras retain the properties of the individual functional domains of the respective nuclear receptors from which the chimeras were generated.

[0152] The carboxy-terminal activation subdomain is in close three-dimensional proximity in the LBD to the ligand, so as to allow for ligands bound to the LBD to coordinate (or interact) with amino acid(s) in the activation subdomain. As described herein, the LBD of a nuclear receptor can be expressed, crystallized, its three dimensional structure determined with a ligand bound (either using crystal data from the same receptor or a different receptor or a combination thereof), and computational methods used to design ligands to its LBD, particularly ligands that contain an extension moiety that coordinates the activation domain of the nuclear receptor.

[0153] The LBD is the second most highly conserved domain in these receptors. As its name suggests, the LBD binds ligands. With many nuclear receptors, including GR, binding of the ligand can induce a conformational change in the LBD that can, in turn, activate transcription of certain target genes. Whereas integrity of several different LBD sub-domains is important for ligand binding, truncated molecules containing only the LBD retain normal ligand-binding activity. This domain also participates in other functions, including dimerization, nuclear translocation and transcriptional activation, as described herein.

[0154] Nuclear receptors usually have HSP binding domains that present a region for binding to the LBD and can be modulated by the binding of a ligand to the LBD. For many of the nuclear receptors ligand binding induces a dissociation of heat shock proteins such that the receptors can form dimers in most cases, after which the receptors bind to DNA and regulate transcription. Consequently, a ligand that stabilizes the binding or contact of the heat shock protein binding domain with the LBD can be designed using the computational methods described herein.

[0155] With the receptors that are associated with the HSP in the absence of the ligand, dissociation of the HSP results in dimerization of the receptors. Dimerization is due to receptor domains in both the DBD and the LBD. Although the main stimulus for dimerization is dissociation of the HSP, the ligand-induced conformational changes in the receptors can have an additional facilitative influence. With the receptors that are not associated with HSP in the absence of the ligand, particularly with the TR, ligand binding can affect the pattern of dimerization. The influence depends on the DNA binding site context, and can also depend on the promoter context with respect to other proteins that can interact with the receptors. A common pattern is to discourage monomer formation, with a resulting preference for heterodimer formation over dimer formation on DNA.

[0156] Nuclear receptor LBDs usually have dimerization domains that present a region for binding to another nuclear receptor and can be modulated by the binding of a ligand to the LBD. Consequently, a ligand that disrupts the binding or contact of the dimerization domain can be designed using the computational methods described herein to produce a partial agonist or antagonist.

[0157] The amino terminal domain of GR is the least conserved of the three domains. This domain is involved in transcriptional activation and, its uniqueness might dictate selective receptor-DNA binding and activation of target genes by GR subtypes. This domain can display synergistic and antagonistic interactions with the domains of the LBD.

[0158] The DNA binding domain has the most highly conserved amino acid sequence among the GR domains. It typically comprises about 70 amino acids that fold into two zinc finger motifs, wherein a zinc atom coordinates four cysteines. The DBD comprises two perpendicularly oriented α -helices that extend from the base of the first and second zinc fingers. The two zinc fingers function in concert along with non-zinc finger residues to direct the GR to specific target sites on DNA and to align receptor dimer interfaces. Various amino acids in the DBD influence spacing between two half-sites (which usually comprises six nucleotides) for receptor dimerization. The optimal spacings facilitate cooperative interactions between DBDs, and D box residues are part of the dimerization interface. Other regions of the DBD facilitate DNA-protein and protein-protein interactions are involved in dimerization.

[0159] In nuclear receptors that bind to a HSP, the ligand-induced dissociation of HSP with consequent dimer formation allows, and therefore, promotes DNA binding. With receptors that are not associated (as in the absence of ligand), ligand binding tends to stimulate DNA binding of heterodimers and dimers, and to discourage monomer binding

to DNA. However, with DNA containing only a single half site, the ligand tends to stimulate the receptor's binding to DNA. The effects are modest and depend on the nature of the DNA site and probably on the presence of other proteins that can interact with the receptors. Nuclear receptors usually have DBD (DNA binding domains) that present a region for binding to DNA and this binding can be modulated by the binding of a ligand to the LBD.

[0160] The modularity of the members of the nuclear receptor superfamily permits different domains of each protein to separately accomplish different functions, although the domains can influence each other. The separate function of a domain is usually preserved when a particular domain is isolated from the remainder of the protein. Using conventional protein chemistry techniques a modular domain can sometimes be separated from the parent protein. By employing conventional molecular biology techniques each domain can usually be separately expressed with its original function intact or chimerics of two different nuclear receptors can be constructed, wherein the chimerics retain the properties of the individual functional domains of the respective nuclear receptors from which the chimerics were generated.

[0161] Various structures have indicated that most nuclear receptor LBDs adopt the same general folding pattern. This fold consists of 10-12 alpha helices arranged in a bundle, together with several beta-strands, and linking segments. A preferred GR α LBD structure of the present invention has 10-11 helices, depending on whether helix-3' is counted. Structural studies have shown that most of the alpha-helices and beta-strands have the same general position and orientation in all nuclear receptor structures, whether ligand is bound or not. However, the AF2 helix has been found in different positions and orientations relative to the main bundle, depending on the presence or absence of the ligand, and also on the chemical nature of the ligand. These structural studies have suggested that many nuclear receptors share a common mechanism of activation, where binding of activating ligands helps to stabilize the AF2 helix in a position and orientation adjacent to helices-3, -4, and -10, covering an opening to the ligand binding site. This position and orientation of the AF2 helix, which will be called the "active conformation", creates a binding site for co-activators. See, e.g., Nolte et al., (1998) *Nature* 395:137-43; Shiau et al., (1998) *Cell* 95: 927-37. This co-activator binding site has a central lipophilic pocket that can accommodate leucine side-chains from co-activators, as well as a "charge-clamp" structure consisting essentially of a lysine residue from helix-3 and a glutamic acid residue from the AF2 helix.

[0162] Structural studies have shown that co-activator peptides containing the sequence LXXLL (SEQ ID NO: 10) (where L is leucine and X can be a different amino acid in different cases) can bind to this co-activator binding site by making interactions with the charge clamp lysine and glutamic acid residues, as well as the central lipophilic region. This co-activator binding site is disrupted when the AF2 helix is shifted into other positions and orientations. In PPAR γ , activating ligands such as rosiglitazone (BRL49653) make a hydrogen bonding interaction with tyrosine-473 in the AF2 helix. Nolte et al., (1998) *Nature* 395:137-43; Gampe et al., (2000) *Mol. Cell* 5: 545-55. Similarly, in GR, the dexamethasone ligand makes van der Waals interaction with the side chain of leucine-753 from the AF2 helix. This interaction is believed in part to stabilize the AF2 helix in the active conformation, thereby allowing co-activators to bind and thus activating transcription from target genes.

[0163] With certain antagonist ligands, or in the absence of any ligand, the AF2 helix can be held less tightly in the active conformation, or can be free to adopt other conformations. This would either destabilize or disrupt the co-activator binding site, thereby reducing or eliminating co-activator binding and transcription from certain target genes. Some of the functions of the GR protein depend on having the full-length amino acid sequence and certain partner molecules, such as co-activators and DNA. However, other functions, including ligand binding and ligand-dependent conformational changes, can be observed experimentally using isolated domains, chimeras and mutant molecules.

[0164] As described herein, the LBD of a GR can be mutated, expressed, crystallized, its three dimensional structure can be determined with a ligand (e.g. fluticasone propionate) bound as disclosed in the present invention. Computational methods can then be employed to design ligands to nuclear receptors, preferably to steroid receptors, and more preferably to glucocorticoid receptors.

IV. The Fluticasone Ligand

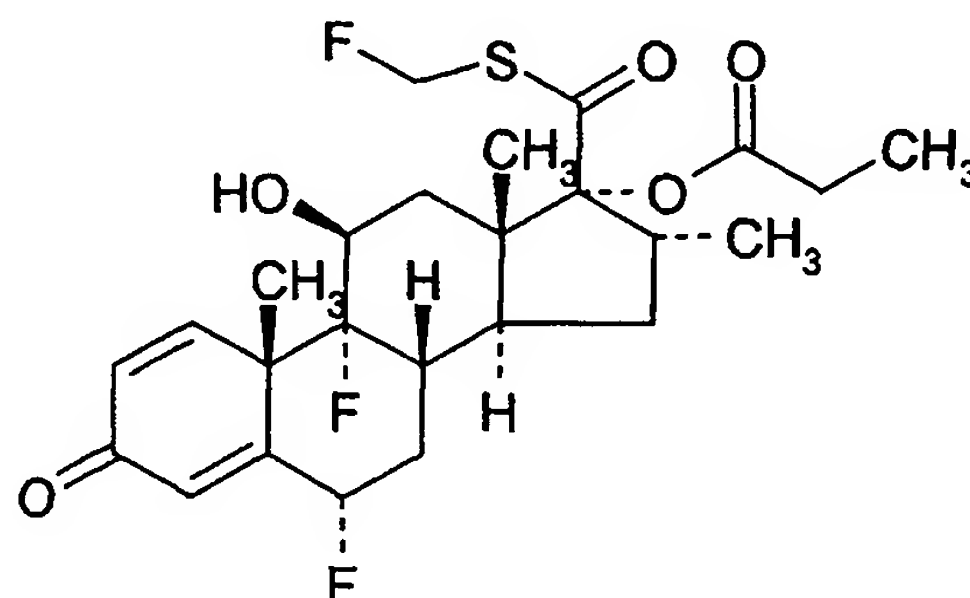
[0165] Ligand binding can induce transcriptional activation functions in a variety of ways. One way is through the dissociation of the HSP from receptors. This dissociation, with consequent dimerization of the receptors and their binding to DNA or other proteins in the nuclear chromatin, allows transcriptional regulatory properties of the receptors to be manifest. This can be especially true of such functions on the amino terminus of the receptors.

[0166] Another way is by altering the receptor to interact with other proteins involved in transcription. These can be proteins that interact directly or indirectly with elements of the proximal promoter or proteins of the proximal promoter. Alternatively, the interactions can be through other transcription factors that themselves interact directly or indirectly with proteins of the proximal promoter. Several different proteins have been described that bind to the receptors in a ligand-dependent manner. In addition, it is possible that in some cases, the ligand-induced conformational changes do not affect the binding of other proteins to the receptor, but do affect their abilities to regulate transcription.

[0167] In one aspect of the present invention, a GR LBD was co-crystallized with a TIF2 peptide and the ligand fluticasone propionate. U.S. Patent No. 4,335,121 to Phillips et al., incorporated herein by reference, teaches an an-

tiinflammatory steroid compound known by the chemical name (6 α , 11 β , 16 α , 17 α)-6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy)androsta-1,4-diene-17-carbothioic acid S-(fluoromethyl) ester and the generic name "fluticasone propionate." Fluticasone propionate in aerosol form, has been accepted by the medical community as useful in the treatment of asthma (see, e.g., Nimmagadda et al., (1998) *Ann. Allerg. Asthma Im.* 81:35-40) and is marketed under the trademarks FLOVENT® and FLONASE®. Fluticasone propionate can also be used in the form of a physiologically acceptable solvate.

[0168] Fluticasone propionate has the chemical structure:



V. The TIF2 Co-activator

[0169] A peptide from the nuclear receptor co-activator TIF2 (SEQ ID NO: 9) was co-crystallized in one aspect of the present invention. Structurally, the nuclear receptor coactivator TIF2 comprises one domain that reacts with a nuclear receptor (nuclear receptor interaction domain, abbreviated "NID") and two autonomous activation domains, AD1 and AD2 (Voegel et al., (1998) *EMBO J.* 17: 507-519). The TIF2 NID comprises three NR-interacting modules, with each module comprising the motif, LXXLL (SEQ ID NO: 10) (Voegel et al., (1998) *EMBO J.* 17: 507-519). Mutation of the motif abrogates TIF2's ability to interact with the ligand-induced activation function-2 (AF-2) found in the ligand-binding domains (LBDs) of many NRs. Presently, it is thought that TIF2 AD1 activity is mediated by CREB binding protein (CBP), however, TIF2 AD2 activity does not appear to involve interaction with CBP (Voegel et al., (1998) *EMBO J.* 17: 507-519).

[0170] In the present invention, residues 740-753 of the TIF2 protein (SEQ ID NO: 9) were co-crystallized with GR and fluticasone propionate. These residues comprise the LXXLL (SEQ ID NO: 10) of AD-2, the third motif in the linear sequence of TIF2. The TIF2 fragment is 13 residues in length and was synthesized using an automated peptide synthesis apparatus. SEQ ID NO: 9, and other sequences corresponding to TIF2 and other co-activators and co-repressors, can be similarly synthesized using automated apparatuses.

VI. Production of GR and Other NR Polypeptides

[0171] In a preferred embodiment, the present invention provides for the first time a GR/TIF2/FP complex. The GR LBD polypeptide of the present invention is expressed as a soluble polypeptide in bacteria, more preferably, in *E. coli*. The GR polypeptides of the present invention, disclosed herein, can thus now provide a variety of host-expression vector systems to express an NR coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing an NR coding sequence; yeast transformed with recombinant yeast expression vectors containing an NR coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing an NR coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing an NR coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities. Methods for constructing expression vectors that comprise a partial or the entire native or mutated NR and GR polypeptide coding sequence and appropriate transcriptional/translational control signals include *in vitro* recombinant DNA techniques, synthetic techniques and *in vivo* recombination/genetic recombination. See, for example, the techniques described throughout Sambrook et al., (1989) *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Laboratory, New York, and Ausubel et al., (1989) *Current Protocols in Molecular Biology*, Greene Publishing Associates and Wiley Interscience, New York, both incorporated herein in their entirety.

[0172] Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, can be used in the expression vector. For example, when cloning

in bacterial systems, inducible promoters such as pL of bacteriophage λ , plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like can be used. When cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter can be used. When cloning in plant cell systems, promoters derived from the genome of plant cells, such as heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) can be used. When cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) can be used. When generating cell lines that contain multiple copies of the tyrosine kinase domain DNA, SV40-, BPV- and EBV-based vectors can be used with an appropriate selectable marker.

[0173] Adequate levels of expression of nuclear receptor LBDs can be obtained by the novel approaches described herein. High level expression in *E. coli* of ligand binding domains of TR and other nuclear receptors, including members of the steroid/thyroid receptor superfamily, such as the estrogen (ER), androgen (AR), mineralocorticoid (MR), progesterone (PR), RAR, RXR and vitamin D (VDR) receptors can also be achieved after review of the expression of a soluble GR polypeptide in bacteria, more preferably, *E. coli* disclosed herein. The GR polypeptides of the present invention, disclosed herein, can thus now provide a variety of host-expression vector systems. Yeast and other eukaryotic expression systems can be used with nuclear receptors that bind heat shock proteins since these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. In a preferred embodiment of the present invention, as disclosed in the Examples, a GR LBD is expressed in *E. coli*.

[0174] Representative nuclear receptors or their ligand binding domains have been cloned and sequenced, including human RAR α , human RAR γ , human RXR α , human RXR β , human PPAR α , human PPAR β or δ (delta), human PPAR γ , human VDR, human ER (as described in Seielstad et al., (1995) *Mol. Endocrinol.* 9: 647-658), human GR, human PR, human MR, and human AR. The ligand binding domain of each of these nuclear receptors has been identified. Using this information in conjunction with the methods described herein, one of ordinary skill in the art can express and purify LBDs of any of the nuclear receptors, bind it to an appropriate ligand, and crystallize the nuclear receptor's LBD with a bound ligand, if desired.

[0175] Extracts of expressing cells are a suitable source of receptor for purification and preparation of crystals of the chosen receptor. To obtain such expression, a vector can be constructed in a manner similar to that employed for expression of the rat TR alpha (Apriletti et al., (1995) *Protein Express. Purif.* 6: 368-370). The nucleotides encoding the amino acids encompassing the ligand binding domain of the receptor to be expressed can be inserted into an expression vector such as the one employed by Apriletti et al. (1995). Stretches of adjacent amino acid sequences can be included if more structural information is desired.

[0176] The native and mutated nuclear receptors in general, and more particularly SR and GR polypeptides, and fragments thereof, of the present invention can also be chemically synthesized in whole or part using techniques that are known in the art (See, e.g., Creighton, (1983) *Proteins: Structures and Molecular Principles*, W.H. Freeman & Co., New York, United States of America, incorporated herein in its entirety).

[0177] In a preferred embodiment, the present invention provides for the first time a soluble GR/TIF2/FP complex. The GR LBD polypeptide of the present invention is expressed as a soluble polypeptide in bacteria, more preferably, *E. coli*, and can be subsequently purified therefrom. Representative purification techniques are also disclosed in the Laboratory Examples, particularly Laboratory Examples 1 and 2. The GR polypeptides of the present invention, disclosed herein, can thus now provide the ability to employ additional purification techniques for both liganded and unliganded NRs. Thus, it is envisioned, based upon the disclosure of the present invention, that purification of the unliganded or liganded NR receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (e.g., HPLC employing a reversed phase column), ion exchange chromatography (e.g., HPLC employing an IEC column), and heparin affinity chromatography. To achieve higher purification for improved crystals of nuclear receptors it is sometimes preferable to ligand shift purify the nuclear receptor using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, the receptor then elutes at the position of the liganded receptor and is removed by the original column run with the unliganded receptor. Typically, saturating concentrations of ligand can be used in the column and the protein can be preincubated with the ligand prior to passing it over the column.

[0178] More recently developed methods involve engineering a "tag" such as a plurality of histidine residues placed on an end of the protein, such as on the amino terminus, and then using a nickel chelation column for purification. See Janknecht, (1991) *Proc. Natl. Acad. Sci. U.S.A.* 88: 8972-8976 (1991), incorporated herein by reference.

VII. Formation of NR Ligand Binding Domain Crystals

[0179] In one embodiment, the present invention provides crystals of GR α LBD. In a preferred embodiment, crystals are obtained using the methodology disclosed in the Laboratory Examples hereinbelow. In this embodiment, the GR α

LBD crystals, which can be native crystals, derivative crystals or co-crystals, have hexagonal unit cells (a hexagonal unit cell is a unit cell wherein $a = b \neq c$, and wherein $\alpha = \beta = 90^\circ$, and $\gamma = 120^\circ$) and space group symmetry $P6_1$. There are two GR α LBD molecules and two TIF2 peptides in the asymmetric unit. In this GR α crystalline form, the unit cell has dimensions of $a = b = 127.656 \text{ \AA}$, $c = 87.725 \text{ \AA}$, and $\alpha = \beta = 90^\circ$, and $\gamma = 120^\circ$. This crystal form can be formed in a crystallization reservoir as described in the Laboratory Examples hereinbelow.

VII.A. Preparation of NR Crystals

[0180] The native and derivative co-crystals, and fragments thereof, disclosed in the present invention can be obtained by a variety of techniques, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see, e.g., McPherson, (1982) *Preparation and Analysis of Protein Crystals*, John Wiley, New York; McPherson, (1990) *Eur. J. Biochem.* 189:1-23; Weber, (1991) *Adv. Protein Chem.* 41:1-36). In a preferred embodiment, the vapor diffusion and hanging drop methods are used for the crystallization of NR polypeptides and fragments thereof. A more preferred hanging drop method technique is disclosed in the Laboratory Examples.

[0181] In general, native crystals of the present invention are grown by dissolving substantially pure NR polypeptide or a fragment thereof in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

[0182] In one embodiment of the invention, native crystals are grown by vapor diffusion (see, e.g., McPherson, (1982) *Preparation and Analysis of Protein Crystals*, John Wiley, New York; McPherson, (1990) *Eur. J. Biochem.* 189:1-23). In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, less than about 25 μL of NR polypeptide solution is mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of the reservoir. The sealed container is allowed to stand until crystals grow. Crystals generally form within two to six weeks, and are suitable for data collection within approximately seven to ten weeks. Of course, those of skill in the art will recognize that the above-described crystallization procedures and conditions can be varied.

VII.B. Preparation of Derivative Crystals

[0183] Derivative crystals of the present invention, e.g. heavy atom derivative crystals, can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. Such derivative crystals are useful for phase analysis in the solution of crystals of the present invention. In a preferred embodiment of the present invention, for example, soaking a native crystal in a solution containing methyl-mercury chloride provides derivative crystals suitable for use as isomorphous replacements in determining the X-ray crystal structure of a NR polypeptide. Additional reagents useful for the preparation of the derivative crystals of the present invention will be apparent to those of skill in the art after review of the disclosure of the present invention presented herein.

VII.C. Preparation of Co-crystals

[0184] Co-crystals of the present invention can be obtained by soaking a native crystal in mother liquor containing compounds known or predicted to bind a NR polypeptide or a fragment thereof (including a NR LBD polypeptide or a fragment thereof). Alternatively, co-crystals can be obtained by co-crystallizing a NR polypeptide or a fragment thereof (including a NR LBD polypeptide or fragment thereof) in the presence of one or more compounds known or predicted to bind the polypeptide. In a preferred embodiment, as disclosed in the Examples, such a compound is fluticasone propionate.

VII.D. Solving a Crystal Structure of the Present Invention

[0185] Crystal structures of the present invention can be solved using a variety of techniques including, but not limited to, isomorphous replacement, anomalous scattering or molecular replacement methods. Computer software packages are also helpful in solving a crystal structure of the present invention. Applicable software packages include but are not limited to the CCP4 package disclosed in the Examples, the X-PLOR™ program (Brünger, (1992) *X-PLOR, Version 3.1. A System for X-ray Crystallography and NMR*, Yale University Press, New Haven, Connecticut; X-PLOR is available from Accelrys of San Diego, California, United States of America, Xtal View (McRee, (1992) *J. Mol. Graphics* 10: 44-46; X-tal View is available from the San Diego Supercomputer Center). SHELXS 97 (Sheldrick, (1990) *Acta Cryst. A* 46: 467; SHELX 97 is available from the Institute of Inorganic Chemistry, Georg-August-Universität, Göttingen, Germany), HEAVY (Terwilliger, Los Alamos National Laboratory) and SHAKE-AND-BAKE (Hauptman, (1997) *Curr. Opin. Struct.*

Biol. 7: 672-80; Weeks et al., (1993) *Acta Cryst. D* 49: 179; available from the Hauptman-Woodward Medical Research Institute, Buffalo, New York) can be used. See also, Ducruix & Geige. (1992) *Crystallization of Nucleic Acids and Proteins: A Practical Approach*. IRL Press, Oxford, England, and references cited therein.

VIII. Characterization and Solution of a GR Ligand Binding Domain Crystal

[0186] The ligand binding domains of many nuclear receptors share a degree of identity with one another. This observation can be beneficial to the characterization and solution of a NR crystal in general and a GR LBD crystal in particular. It is also noted that, within the ligand binding domains (LBDs), the sequence identity there is a degree of homology, which is summarized in the following table:

Sequence Identity of NR LBDs				
	GR	MR	PR	AR
GR	100%	56%	54%	50%
MR	56%	100%	55%	51%
PR	54%	55%	100%	55%
AR	50%	51%	55%	100%

[0187] Turning to Figure 17, a figure depicting a sequence alignment of several NRs, this figure depicts structural and sequence homology between the several NRs, as well as similarities in the overall protein architecture. In Figure 17, secondary structures in GR, PR and AR are indicated by large boxes and by annotation underneath the sequences. The secondary structure attributed to MR is that demonstrated by a homology model of the present invention, as discussed hereinbelow and in the Laboratory Examples. For each line of the alignment, the three-digit number provides the residue number of the first residue in the line. Residues within 5.0 angstroms distance of a bound ligand are identified with small boxes. The bound ligands are FP, progesterone and dihydrotestosterone for GR, PR and AR, respectively, and subunit A was used for the distance calculations in all three cases. Three residues in GR, Met639, Cys643 and Phe740, lie within 5.0 angstroms distance to FP in the GR/FP structure, but do not lie within 5.0 angstroms distance to Dex in the GR/Dex structure. These three residues are denoted in Figure 17 by underlining. Met639 and Cys643 interact with the propionate group in FP, as shown in the schematic diagrams of Figures 8A and 8B, and are involved in the expanded ligand binding pocket. Phe740 lies approximately 5 angstroms from the F-CH₂-thioester group of FP, but fails to make any significant interaction, and is not shown in either of the schematic diagrams of Figures 8A and 8B.

[0188] This information, combined with the structural features observed in a GR/FP structure of the present invention, as discussed herein below, can facilitate the design of additional modulators of GR. Such modulators can comprise FP derivatives, which are preferred modulators.

VIII.A Unique Structural Features of the GR/FP/TF2 Structure

[0189] The structure of GR in complex with fluticasone propionate and a TIF2 co-activator peptide reveals several features of the GR structure that, prior to the present disclosure, have not been observed or reported. The detailed structural information about the GR LBD and the expanded binding pocket provided herein can be further exploited to design receptor specific agonists or antagonists.

[0190] One unique feature of the GR α /FP/TIF2 structure relates to the conformation of the GR expanded binding pocket observed when GR binds FP. The GR/FP/TIF2 crystal structure is a significant and unique addition to the knowledge of the three-dimensional structure of the GR and of the associated changes in that structure as a result of the binding of various glucocorticoids. As evidenced in the GR/TIF2/FP crystal structure, the binding of FP induces a conformational change in the GR protein that opens additional volume into which the propionate side chain of FP extends, leading to an expanded binding pocket. The identification of the expanded binding pocket facilitates the ability to better interpret and explain the structure-activity relationship (SAR) observed for both steroidal and non-steroidal glucocorticoids. Thus, the GR/FP/TIF2 crystal structures disclosed herein can be employed to further explain glucocorticoid binding and GR's functional activity via an analysis of compounds as they occupy the added volume of the expanded binding pocket.

VIII.A.1. The Overall Structure of the GR/TF2/FP Complex

[0191] The GR/TIF2/fluticasone propionate complex of the present invention crystallized in the P6₁ space group with two complexes in each asymmetry unit. Data was collected from a single crystal to a resolution of 2.6 Å. The structure

was solved using the molecular replacement method. A GR/TIF2/dexamethasone structure was used as the initial search model (see Laboratory Example 5). The electron density map calculated with the molecular replacement solutions showed clear tracings for two GR LBD monomers (GR residues 521-777), the LXXLL motifs (SEQ ID NO: 10) of two TIF2 peptides, and two bound molecules of fluticasone propionate (see Figure 2). The statistics of data sets and the refined structures are summarized in Table 1.

[0192] In a preferred embodiment of the crystals, the two GR LBD monomers in each asymmetry unit are packed into a symmetric dimer. Each GR LBD is bound with a molecule of fluticasone propionate and a TIF2 coactivator peptide (see Figure 2). The structure of the GR LBD contains 11 α -helices and 4 small β -strands that fold into a three-layer helical domain with an overall organization closely resembling the structures of PR and AR (Matias et al., (2000) *J. Biol. Chem.* 275:26164-26171; Sack et al., (2001) *Proc. Natl. Acad. Sci.* 98:4904-4909; Williams & Sigler, (1998) *Nature* 393:392-396). Helices 1 and 3 form one side of a helical sandwich whereas helices 7 and 10 form the other side. The middle layer of helices (helices 4, 5, 8, and 9) are present in the top half of the protein but are absent in the bottom half of the protein. This arrangement of helices thus creates a cavity in the bottom half of the GR LBD where the fluticasone propionate is bound, and forms an element of an expanded binding pocket. The conformation adopted by FP in the binding pocket is depicted in Figure 3. Figure 3 shows the propionate moiety and the space it occupies in the expanded binding pocket.

[0193] The AF-2 helix, which plays an essential function of ligand-dependent activation, adopts the so-called active or "agonist-bound" conformation that is packed against helices 3, 4, and 10 as an integrated part of the domain structure. Following the AF-2 helix is an extended strand that forms a conserved beta sheet with a β -strand between helices 8 and 9. The LLRYLL sequence (SEQ ID NO: 11) in the TIF2 motif forms a two-turn α -helix that docks the hydrophobic leucine side chains into a groove formed in part by the AF-2 helix and residues from helices 3, 3', 4 and 5 (see Figure 2). Both ends of the coactivator helix are clamped by E754 on the AF-2 helix and K579 on helix 3, respectively. This mode of coactivator binding further stabilizes the overall GR LBD structure and the arrangement of the dimer configuration.

VIII.A.2. Differences Between the GR/TIF2/FP Complex and a GR/Dex/TIF2 Complex

[0194] Although the GR/TIF2/FP complex is similar to the GR/TIF2/dexamethasone complex ("the Dex structure"; coordinates of this structure are presented in Table 3), there are a number of differences in their crystallization conditions and their detailed structures. First, the FP complex contains a TIF2 peptide that is 10 residues shorter than the TIF2 peptide used in the GR/TIF2/Dex complex. The crystals of the GR/TIF2/FP complex were obtained using MgSO_4 as precipitant, whereas ammonium formate was used to obtain crystals of the GR/TIF2/Dex complex. The crystallization conditions for the GR/TIF2/Dex complex were not preferred for the GR/TIF2/FP complex.

[0195] Second, despite the similar LBD structure and arrangement of the dimer configuration between the FP and the Dex structures, there is a dramatic difference in the ligand binding pocket that is occupied by the propionate group of the fluticasone. This ligand binding pocket is much smaller in size in the GR/Dex structure. Although the 17- α -hydroxyl of dexamethasone points toward this region of the ligand binding pocket, the volume of this ligand binding pocket is largely unoccupied in the Dex structure. The volume of the ligand binding pocket in the FP structure is significantly expanded to accommodate the larger propionate group of fluticasone in both LBD monomers of the dimer, and forms an expanded binding pocket. This expansion in the volume of the ligand binding pocket in the GR/TIF2/FP structure, as compared with the GR/TIF2/Dex structure, is readily seen when Figures 5A and 5B, showing the available pocket volume in the GR/Dex structure, are compared with Figures 6A and 6B, showing the available pocket volume in the GR/TIF2/FP structure. The expanded binding pocket of the FP structure is also depicted in Figure 7A and 7B, where the additional pocket volume of the FP structure over that of the Dex structure is represented by a semi-transparent surface.

[0196] Referring again to Figure 5A, this figure depicts subunit A, and shows dexamethasone, selected side-chains from the protein, and a semi-transparent surface enclosing the volume that is available to oxygen-sized ligand atoms within the ligand binding region of the GR protein in the GR/Dex structure. Figure 5B depicts subunit B, and shows the corresponding ligand molecule, side-chains and pocket volume from subunit B of the same GR/Dex structure. Protein side-chains are depicted with ball and stick representation, using thin sticks and small balls. The dexamethasone ligand is also depicted by a ball and stick representation, but using thicker sticks and larger balls. The pocket volume is depicted by a surface generated over closely-spaced spheres within the pocket of the GR/Dex structure. The spheres have radius 1.4 angstroms, and are arranged on a rectangular grid with a spacing of 0.3 angstroms. The surface is a "quick" surface generated within the INSIGHTII molecular graphics program using the "very high" surface quality. Atoms are represented by various shades of gray, with carbon darker than nitrogen, which is darker than oxygen, which is darker than sulfur. Fluorine is represented by a shade similar to nitrogen, but can be distinguished from nitrogen because the protein has no fluorine atoms, and the dexamethasone molecule has no nitrogens. The shades of gray are further modified by the use of depth queueing to help distinguish foreground and background features.

[0197] Turning next to Figure 6A, this figure depicts GR subunit A, and shows FP, selected side-chains from the protein, and a semi-transparent surface enclosing the volume that is available to oxygen-sized ligand atoms within the ligand binding region of the GR protein in the GR/TIF2/FP structure. Figure 6B depicts GR subunit B, showing the corresponding ligand molecule, side-chains and pocket volume from GR subunit B of the same GR/TIF2/FP structure. This figure was generated using the same methods as Figures 5A and 5B and uses the same representation and shading for atoms and volumes.

[0198] Figure 7A depicts GR GR subunit A, and shows FP, selected side-chains from the protein in the GR/FP/TIF2 structure, and a semi-transparent surface enclosing the "extra volume" that is available in the GR/FP ligand binding pocket, but not in the GR/Dex ligand binding pocket. This "extra" volume is essentially the volume depicted in Figure 5A subtracted from the volume depicted in Figure 6A and contributes to the expanded binding pocket observed in the GR/TIF2/FP structure. The available volumes in the structures were represented computationally by a collection of closely-spaced water-sized spheres. The extra volume in the GR/TIF2/FP structure was identified computationally by comparing these two collections of water-sized spheres, represented by a collection of closely-spaced spheres of radius 0.2 angstroms, and then depicted by generation of the semi-transparent surface.

[0199] Figure 7B depicts GR subunit B, and shows the corresponding ligand molecule, side-chains and "extra volume" from GR subunit B. The representation and shading for atoms is the same as Figures 5A and 5B above. The "extra volume" is depicted by a surface generated over closely-space spheres occupying the region of the GR/TIF2/FP pocket, (see Figures 6A and 6B), that is not available in the GR/Dex structure, (see Figures 5A and 5B). The spheres used for the surface calculation have a radius of 0.2 angstroms, and are arranged on a rectangular grid with a spacing of 0.3 angstroms.

[0200] Figure 8A is a schematic representation of molecular interactions between the bound FP ligand and residues in the GR protein in subunit A. The dashed lines depict most of the significant interactions of 5.0 angstroms or less, although several of the less important interactions have been omitted for clarity. The propionate side-chain adopts different conformations in the two subunits, and the approximate conformation in subunit A is depicted schematically here. Several side-chains in the protein adopt different conformations in the two subunits. While these side-chain conformations are not represented explicitly, their interactions with the ligand, and differences in these interactions in GR subunits A and B, are represented.

[0201] Figure 8B is a schematic representation of molecular interactions between the bound FP ligand and residues in the GR protein in GR subunit B. The dashed lines depict most of the significant interactions of 5.0 angstroms or less, although several of the less important interactions have been omitted for clarity. The propionate side-chain adopts different conformations in the two subunits, and the approximate conformation in GR subunit B is depicted schematically in Figure 8B.

[0202] There are no large conformational changes of helices or loops between the FP and Dex structures, consistent with the observation that both ligands bound with high affinity. Instead, the larger expanded binding pocket in the FP structure is formed by gently pushing out helices 3, 6, 7 and 10 and the loop preceeding the AF-2 helix, which make up the framework of the ligand binding pocket (see Figure 4). The subtle changes in the conformation of these helices and loops in the FP structure, which are highlighted in Figure 4 by arrows, would be difficult to predict by modeling the GR/TIF2/Dex structure.

[0203] The expanded binding pocket is surrounded by side chains of more than 10 residues, including M560, L563, F623, M639, Q642, M643, M646, Y735, C736, T739 and 1747. Conformations of these side chains generally favor formation of the larger expanded binding pocket in the FP structure. By way of example, in order to assume the observed positions, residues Q642 and Y735 in monomer B undergo a large conformational changes. Residue Q642, on the other hand, flips out of pocket to the space that is normally occupied by Y735. The conformational changes of these two residues contribute to an expanded binding pocket in this LBD monomer (see Table 2). The expanded binding pocket in the FP structure is a feature making the present invention distinct from known GR structures (e.g. the GR/TIF2/Dex structure, atomic coordinates of which are presented in Table 3) and offers several advantages for structure-based drug discovery over the use of the GR/TIF2/Dex structure.

VIII.E. Generation of Easily-Solved NR Crystals

[0204] The present invention discloses a substantially pure GR LBD polypeptide in crystalline form. In a preferred embodiment, exemplified in the Figures and Laboratory Examples, GR α is crystallized with a bound ligand and a bound co-activator peptide. Crystals can be formed from NR LBD polypeptides that are usually expressed by a cell culture, such as *E. coli*. Bromo- and iodo-substitutions can be included during the preparation of crystal forms and can act as heavy atom substitutions in GR ligands and crystals of NRs. This method can be advantageous for the phasing of the crystal, which is a crucial, and sometimes limiting, step in solving the three-dimensional structure of a crystallized entity. Thus, the need for generating the heavy metal derivatives traditionally employed in crystallography can be eliminated. After the three-dimensional structure of a NR or an NR LBD with or without a ligand and/or a co-activator bound is

determined, the resultant three-dimensional structure can be used in computational methods to design synthetic ligands for a NR and for other NR polypeptides. Further activity structure relationships can be determined through routine testing employing assays disclosed herein and known in the art.

IX. Uses of NR Crystals and the Three-Dimensional Structure of the Ligand Binding Domain of GR α

[0205] The solved crystal structure of the present invention is useful in the design of modulators of activity mediated by the glucocorticoid receptor and by other nuclear receptors. Evaluation of the available sequence data shows that GR α is particularly similar to MR, PR and AR. The GR α LBD has approximately 56%, 54% and 50% sequence identity to the MR, PR and AR LBDs, respectively. The GR β amino acid sequence is identical to the GR α amino acid sequence for residues 1-726, but the remaining 16 residues in GR β show no significant similarity to the remaining 51 residues in GR α .

[0206] The present GR α X-ray structure can also be used to build models for targets where no X-ray structure is available, such as MR. Additionally, targets whose X-ray structures have been solved (e.g. AR and PR), do not comprise an expanded binding pocket. Thus, these previously solved structures cannot be effectively employed in an attempt to model these structures in association with a ligand comprising a large 17 α substituent. By employing a GR α X-ray structure of the present invention, however, such models can be generated. These generated models can aid in the design of compounds to selectively modulate any desired subset of GR α , MR, PR, AR and other related nuclear receptors.

[0207] Various models can be built, such as homology models and docking models. Indeed, homology models of AR, MR and PR form aspects of the present invention. These models incorporate the expanded binding pocket observed in the GR/TIF2/FP structure. Although a few NR structures are available, these structures do not comprise an expanded binding pocket and are therefore of limited use in rational drug design.

IX.A. Design and Development of NR Modulators

[0208] The present invention, particularly the computational methods, can be used to design drugs for a variety of nuclear receptors, such as receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs) and progestins (PRs).

[0209] The knowledge of the structure of the GR α ligand binding domain (LBD), an aspect of the present invention, provides a tool for investigating the mechanism of action of GR α and other NR polypeptides in a subject. For example, various computer modelling programs, as described herein, can predict the binding of various ligand molecules to the LBD of GR β , or another steroid receptor or, more generally, nuclear receptor. Upon discovering that such binding in fact takes place, knowledge of the protein structure then allows design and synthesis of small molecules that mimic the functional binding of the ligand to the LBD of GR α , and to the LBDs of other polypeptides. This is the method of "rational" drug design, further described herein.

[0210] Use of the isolated and purified GR α crystalline structure of the present invention in rational drug design is thus provided in accordance with the present invention. Additional rational drug design techniques are described in U. S. Patent Nos. 5,834,228 and 5,872,011, incorporated herein in their entirety.

[0211] Thus, in addition to the compounds described herein, other sterically similar compounds can be formulated to interact with the key structural regions of an NR, SR or GR in general, or of GR α in particular. The generation of a structural functional equivalent can be achieved by the techniques of modeling and chemical design known to those of skill in the art and described herein. It will be understood that all such sterically similar constructs fall within the scope of the present invention.

IX.A.1. Rational Drug Design

[0212] The three-dimensional structure of a FP bound GR α is unprecedented and will greatly aid in the development of new synthetic ligands for NR polypeptides, such as GR agonists and antagonists, including those that bind exclusively to any one of the GR subtypes. In addition, NRs are well suited to modern methods, including three-dimensional structure elucidation and combinatorial chemistry, such as those disclosed in U.S. Patent Nos. 5,463,564, and 6,236,946 incorporated herein by reference. Structure determination using X-ray crystallography is possible because of the solubility properties of NRs. Computer programs that use crystallography data when practicing the present invention will enable the rational design of ligands to these receptors.

[0213] Programs such as RASMOL (Biomolecular Structures Group, Glaxo Wellcome Research & Development Stevenage, Hertfordshire, UK Version 2.6, August 1995, Version 2.6.4, December 1998, © Roger Sayle 1992-1999) and Protein Explorer (Version 1.87, July 3, 2001, © Eric Martz, 2001 and available online at <http://www.umass.edu/microbio/chime/explorer/index.htm>) can be used with the atomic structural coordinates from crystals generated by

practicing the invention or used to practice the invention by generating three-dimensional models and/or determining the structures involved in ligand binding. Computer programs such as those sold under the registered trademark IN-SIGHTII® (available from Accelrys of San Diego, California, United States of America) and the programs GRASP (Nicholls et al., (1991) *Proteins* 11: 281) and SYBYL™ (available from Tripos, Inc. of St. Louis, Missouri, United States of America) allow for further manipulations and the ability to introduce new structures. In addition, high throughput binding and bioactivity assays can be devised using purified recombinant protein and modern reporter gene transcription assays known to those of skill in the art in order to refine the activity of a designed ligand.

[0214] A method of identifying modulators of the activity of an NR polypeptide using rational drug design is thus provided in accordance with the present invention. The method comprises designing a potential modulator for an NR polypeptide of the present invention that will form non-covalent interactions with amino acids in the ligand binding pocket based upon the crystalline structure of the GR α LBD polypeptide; synthesizing the modulator; and determining whether the potential modulator modulates the activity of the NR polypeptide. In a preferred embodiment, the modulator is designed for an SR polypeptide. In a more preferred embodiment, the modulator is designed for a GR α polypeptide. Preferably, the GR α polypeptide comprises the amino acid sequence of SEQ ID NOs: 2 and 4 and more preferably, the GR α LBD comprises the amino acid sequence of SEQ ID NOs: 6 and 8. The determination of whether the modulator modulates the biological activity of an NR polypeptide is made in accordance with the screening methods disclosed herein, or by other screening methods known to those of skill in the art. Modulators can be synthesized using techniques known to those of ordinary skill in the art.

[0215] In an alternative embodiment, a method of designing a modulator of an NR polypeptide in accordance with the present invention is disclosed comprising: (a) selecting a candidate NR ligand; (b) determining which amino acid or amino acids of an NR polypeptide interact with the ligand using a three-dimensional model of a crystallized GR α LBD in complex with a co-activator peptide and fluticasone propionate; (c) identifying in a biological assay for NR activity a degree to which the ligand modulates the activity of the NR polypeptide; (d) selecting a chemical modification of the ligand wherein the interaction between the amino acids of the NR polypeptide and the ligand is predicted to be modulated by the chemical modification; (e) synthesizing a chemical compound with the selected chemical modification to form a modified ligand; (f) contacting the modified ligand with the NR polypeptide; (g) identifying in a biological assay for NR activity a degree to which the modified ligand modulates the biological activity of the NR polypeptide; and (h) comparing the biological activity of the NR polypeptide in the presence of modified ligand with the biological activity of the NR polypeptide in the presence of the unmodified ligand, whereby a modulator of an NR polypeptide is designed.

[0216] An additional method of designing modulators of an NR or an NR LBD can comprise: (a) determining which amino acid or amino acids of an NR LBD interacts with a first chemical moiety (at least one) of the ligand using a three dimensional model of a crystallized protein comprising an NR LBD in complex with a bound ligand; and (b) selecting one or more chemical modifications of the first chemical moiety to produce a second chemical moiety with a structure to either decrease or increase an interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the first chemical moiety. A structure disclosed herein, namely a structure comprising a GR α LBD in complex with fluticasone propionate, can be employed in this method. This is a general strategy only, however, and variations on this disclosed protocol would be apparent to those of skill in the art upon consideration of the present disclosure.

[0217] Once a candidate modulator is synthesized as described herein and as will be known to those of skill in the art upon contemplation of the present invention, it can be tested using assays to establish its activity as an agonist, partial agonist or antagonist, and affinity, as described herein. After such testing, a candidate modulator can be further refined by generating LBD crystals with the candidate modulator bound to the LBD. The structure of the candidate modulator can then be further refined using the chemical modification methods described herein for three dimensional models to improve the activity or affinity of the candidate modulator and make second generation modulators with improved properties, such as that of a super agonist or antagonist, as described herein.

IX.A.2. Methods for Using the GR α LBD Structural Coordinates For Molecular Design

[0218] The present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including modulatory compounds, capable of binding to the ligand binding pocket or an accessory binding site of an NR and an NR LBD, in whole or in part. Correspondingly, the present invention also provides for the application of similar techniques in the design of modulators of any NR polypeptide.

[0219] In accordance with a preferred embodiment of the present invention, the structure coordinates of a crystalline GR α LBD in complex with a co-activator and fluticasone propionate can be employed to design compounds that bind to a GR LBD (more preferably a GR α LBD) and alter the properties of a GR LBD (for example, the dimerization ability, ligand binding ability or effect on transcription) in different ways. One aspect of the present invention provides for the design of compounds that can compete with natural or engineered ligands of a GR polypeptide by binding to all, or a portion of, the binding sites on a GR LBD. The present invention also provides for the design of compounds that can

bind to all, or a portion of, an accessory binding site on a GR that is already binding a ligand. Similarly, non-competitive agonists/ligands that bind to and modulate GR LBD activity, whether or not it is bound to another chemical entity, and partial agonists and antagonists can be designed using the GR LBD structure coordinates of this invention.

[0220] A second design approach is to probe an NR or an NR LBD (preferably a GR α or GR α LBD) crystal with molecules comprising a variety of different chemical entities to determine optimal sites for interaction between candidate NR or NR LBD modulators and the polypeptide. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of the site where each type of solvent molecule adheres. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their NR modulator activity. Representative designs are also disclosed in published PCT application WO 99/26966.

[0221] Once a computationally-designed ligand is synthesized using the methods of the present invention or other methods known to those of skill in the art, assays can be used to establish its efficacy of the ligand as a modulator of NR (preferably GR α) activity. After such assays, the ligands can be further refined by generating intact NR or NR LBD crystals with a ligand and/or a co-activator peptide bound to the LBD. The structure of the ligand can then be further refined using the chemical modification methods described herein and known to those of skill in the art, in order to improve the modulation activity or the binding affinity of the ligand. This process can lead to second generation ligands with improved properties.

[0222] Ligands also can be selected that modulate NR responsive gene transcription by the method of altering the interaction of co-activators and co-repressors with their cognate NR. For example, agonistic ligands can be selected that block or dissociate a co-repressor from interacting with a GR, and/or that promote binding or association of a co-activator. Antagonistic ligands can be selected that block co-activator interaction and/or promote co-repressor interaction with a target receptor. Selection can be done via binding assays that screen for designed ligands having the desired modulatory properties. Preferably, interactions of a GR α polypeptide are targeted. A suitable assay for screening that can be employed, *mutatis mutandis* in the present invention, as described in Oberfield et al., (1999) *Proc. Natl. Acad. Sci. U. S. A.* 96(11): 6102-6, incorporated herein in its entirety by reference. Other examples of suitable screening assays for GR function include an *in vitro* peptide binding assay representing ligand-induced interaction with coactivator (Zhou et al., (1998) *Mol. Endocrinol.* 12: 1594-1604; Parks et al., (1999) *Science* 284: 1365-1368) or a cell-based reporter assay related to transcription from a GRE (see Jenkins et al., (2001) *Trends Endocrinol. Metab.* 12: 122-126) or a cell-based reporter assay related to repression of genes driven via NF-kB (DeBosscher et al., (2000) *Proc. Natl. Acad. Sci. U. S. A.* 97: 3919-3924).

IX.A.3. Methods of Designing NR LBD Modulator Compounds

[0223] Knowledge of the three-dimensional structure of the GR LBD complex of the present invention can facilitate a general model for modulator (e.g. agonist, partial agonist, antagonist and partial antagonist) design. Other ligand-receptor complexes belonging to the nuclear receptor superfamily can have a ligand binding pocket similar to that of GR and therefore the present invention can be employed in agonist/antagonist design for other members of the nuclear receptor superfamily and the steroid receptor subfamily. Examples of suitable receptors include those of the NR superfamily and those of the SR and TR subfamilies.

[0224] The design of candidate substances, also referred to as "compounds" or "candidate compounds", that augment or inhibit NR LBD-mediated activity according to the present invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with a NR LBD. Non-covalent molecular interactions important in the association of a NR LBD with its substrate include hydrogen bonding, van der Waals interactions and hydrophobic interactions.

[0225] The interaction between an atom of a LBD amino acid and an atom of an LBD ligand can be made by any force or attraction described in nature. Usually the interaction between the atom of the amino acid and the ligand will be the result of a hydrogen bonding interaction, charge interaction, hydrophobic interaction, van der Waals interaction or dipole interaction. In the case of the hydrophobic interaction it is recognized that this is not a per se interaction between the amino acid and ligand, but rather the usual result, in part, of the repulsion of water or other hydrophilic group from a hydrophobic surface. Reducing or enhancing the interaction of the LBD and a ligand can be measured by calculating or testing binding energies, computationally or using thermodynamic or kinetic methods as known in the art.

[0226] Second, the compound must be able to assume a conformation that allows it to associate with a NR LBD. Although certain portions of the compound might not directly participate in this association with a NR LBD, those portions can still influence the overall conformation of the molecule. This, in turn, can have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., the ligand binding pocket or an accessory binding site of a NR LBD, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with a NR LBD.

[0227] Chemical modifications will often enhance or reduce interactions of an atom of a LBD amino acid and an atom of an LBD ligand. Altering a degree of steric hinderance is one approach that can be employed to alter the interaction of a LBD binding pocket with an activation domain. Chemical modifications are preferably introduced at C-, C-H, and C-OH positions in a ligand, where the carbon is part of the ligand structure that remains the same after modification is complete. In the case of C-H, C could have 1, 2 or 3 hydrogens, but typically only one hydrogen is replaced. An H or OH can be removed after modification is complete and replaced with a desired chemical moiety.

[0228] The potential modulatory or binding effect of a chemical compound on a NR LBD can be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques that employ the coordinates of a crystalline GR α LBD polypeptide of the present invention. If the theoretical structure of the given compound suggests insufficient interaction and association between it and a NR LBD, synthesis and testing of the compound is obviated. However, if computer modeling indicates a strong interaction, the molecule can then be synthesized and tested for its ability to bind and modulate the activity of a NR LBD. In this manner, synthesis of unproductive or inoperative compounds can be minimized or avoided.

[0229] A modulatory or other binding compound of a NR LBD polypeptide (preferably a GR α LBD) can be computationally evaluated and designed via a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with an individual binding site or other area of a crystalline GR α LBD polypeptide of the present invention and to interact with the amino acids disposed in the binding sites.

[0230] Interacting amino acids forming contacts with a ligand and the atoms of the interacting amino acids are usually 2 to 4 angstroms away from the center of the atoms of the ligand. Generally these distances are determined by computer as discussed herein and by McRee (McRee, (1993) Practical Protein Crystallography, Academic Press, New York), however distances can be determined manually once the three dimensional model is made. More commonly, the atoms of the ligand and the atoms of interacting amino acids are 3 to 4 angstroms apart. A ligand can also interact with distant amino acids, after chemical modification of the ligand to create a new ligand. Distant amino acids are generally not in contact with the ligand before chemical modification. A chemical modification can change the structure of the ligand to make as new ligand that interacts with a distant amino acid usually at least 4.5 angstroms away from the ligand. Often distant amino acids will not line the surface of the binding cavity for the ligand, as they are too far away from the ligand to be part of a pocket or surface of the binding cavity.

[0231] A variety of methods can be used to screen chemical entities or fragments for their ability to associate with an NR LBD and, more particularly, with the individual binding sites of an NR LBD, such as ligand binding pocket or an accessory binding site. This process can begin by visual inspection of, for example, the ligand binding pocket on a computer screen based on the GR α LBD atomic coordinates presented in Tables 2-11 as described herein. Selected fragments or chemical entities can then be positioned in a variety of orientations, or docked, within an individual binding site of a GR α LBD as defined herein above. Docking can be accomplished using software programs such as those available under the tradenames QUANTATM (Accelrys of San Diego, California, United States of America) and SYB-TM (Tripos, Inc., St. Louis, Missouri, United States of America), followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARM (Brooks et al., (1983) J. Comp. Chem., 8: 132) and AMBER 5 (Case et al., (1997), AMBER 5, University of California, San Francisco, California, United States of America; Pearlman et al., (1995) Comput. Phys. Commun. 91:1-41).

[0232] Specialized computer programs can also assist in the process of selecting fragments or chemical entities. These include:

1. GRIDTM program, version 17 (Goodford, (1985) J. Med. Chem. 28:849-57), which is available from Molecular Discovery Ltd., Oxford, UK;
2. MCSSTM program (Miranker & Karplus, (1991) Proteins 11:29-34), which is available from Accelrys of San Diego, California, United States of America;
3. AUTODOCKTM 3.0 program (Goodsell & Olsen, (1990) Proteins 8:195-202), which is available from the Scripps Research Institute, La Jolla, California, United States of America;
4. DOCKTM 4.0 program (Kuntz et al., (1992) J. Mol. Biol. 161:269-88), which is available from the University of California, San Francisco, California, United States of America;
5. FLEX-XTM program (See, Rarey et al., (1996) J. Comput. Aid. Mol. Des. 10:41-54), which is available from Tripos, Inc., St. Louis, Missouri, United States of America;
6. MVP program (Lambert, (1997) in Practical Application of Computer-Aided Drug Design, (Charifson, ed.) Marcel-Dekker, New York, New York, United States of America, pp. 243-303); and
7. LUDITM program (Bohm, (1992) J. Comput. Aid. Mol. Des. 6:61-78), which is available from Accelrys of San Diego, California, United States of America.

[0233] Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or modulator. Assembly can proceed by visual inspection of the relationship of the fragments to each other on

the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a GR α LBD. Manual model building using software such as QUANTA™ or SYBYL™ typically follows.

[0234] Useful programs to aid one of ordinary skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT™ program (Bartlett et al., (1989) *Special Pub., Royal Chem. Soc.* 78:182-96), which is available from the University of California, Berkeley, California, United States of America;
2. 3D Database systems, such as MACCS-3D™ system program, which is available from MDL Information Systems, San Leandro, California, United States of America. This area is reviewed in Martin, (1992) *J. Med. Chem.* 35:2145-54; and
3. HOOK™ program (Eisen et al., (1994). *Proteins* 19:199-221), which is available from Accelrys of San Diego, California, United States of America.

[0235] Instead of proceeding to build a GR LBD modulator (preferably a GR α LBD modulator) in a step-wise fashion one fragment or chemical entity at a time as described above, modulatory or other binding compounds can be designed as a whole or *de novo* using the structural coordinates of a crystalline GR α LBD polypeptide of the present invention and either an empty binding site or optionally including some portion(s) of a known modulator(s). Applicable methods can employ the following software programs:

1. LUDI™ program (Bohm, (1992) *J. Comput. Aid. Mol. Des.* 6:61-78), which is available from Accelrys of San Diego, California, United States of America;
2. LEGEND™ program (Nishibata & Itai, (1991) *Tetrahedron* 47:8985); and
3. LEAPFROG™, which is available from Tripos Associates, St. Louis, Missouri, United States of America.

[0236] Other molecular modeling techniques can also be employed in accordance with this invention. See, e.g., Cohen et al., (1990) *J. Med. Chem.* 33: 883-94. See also, Navia & Murcko, (1992) *Curr. Opin. Struc. Biol.* 2: 202-10; U.S. Patent No. 6,008,033, herein incorporated by reference.

[0237] Once a compound has been designed or selected by the above methods, the efficiency with which that compound can bind to a NR LBD can be tested and optimized by computational evaluation. By way of particular example, a compound that has been designed or selected to function as a NR LBD modulator should also preferably traverse a volume not overlapping that occupied by the binding site when it is bound to its native ligand. Additionally, an effective NR LBD modulator should preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient NR LBD modulators should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, and preferably, not greater than 7 kcal/mole. It is possible for NR LBD modulators to interact with the polypeptide in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the modulator binds to the polypeptide.

[0238] A compound designed or selected as binding to an NR polypeptide (preferably a GR α LBD polypeptide) can be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target polypeptide. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the modulator and the polypeptide when the modulator is bound to an NR LBD preferably make a neutral or favorable contribution to the enthalpy of binding.

[0239] Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include:

1. Gaussian 98™, which is available from Gaussian, Inc., Pittsburgh, Pennsylvania, United States of America;
2. AMBER™ program, version 6.0, which is available from the University of California at San Francisco, San Francisco, California, United States of America;
3. QUANTA™ program, which is available from Accelrys of San Diego, California, United States of America;
4. CHARMM® program, which is available from Accelrys of San Diego, California, United States of America; and
5. Insight II® program, which is available from Accelrys of San Diego, California, United States of America.

[0240] These programs can be implemented using a suitable computer system. Other hardware systems and software packages will be apparent to those skilled in the art after review of the disclosure of the present invention presented herein.

[0241] Once an NR LBD modulating compound has been optimally selected or designed, as described above, sub-

stitutions can then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation are preferably avoided. Such substituted chemical compounds can then be analyzed for efficiency of fit to an NR LBD binding site using the same computer-based approaches described in detail above.

IX.B. Design of Modulators Based on the Expanded Binding Pocket of GR Observed in the GR/FP/TIF2 Structure

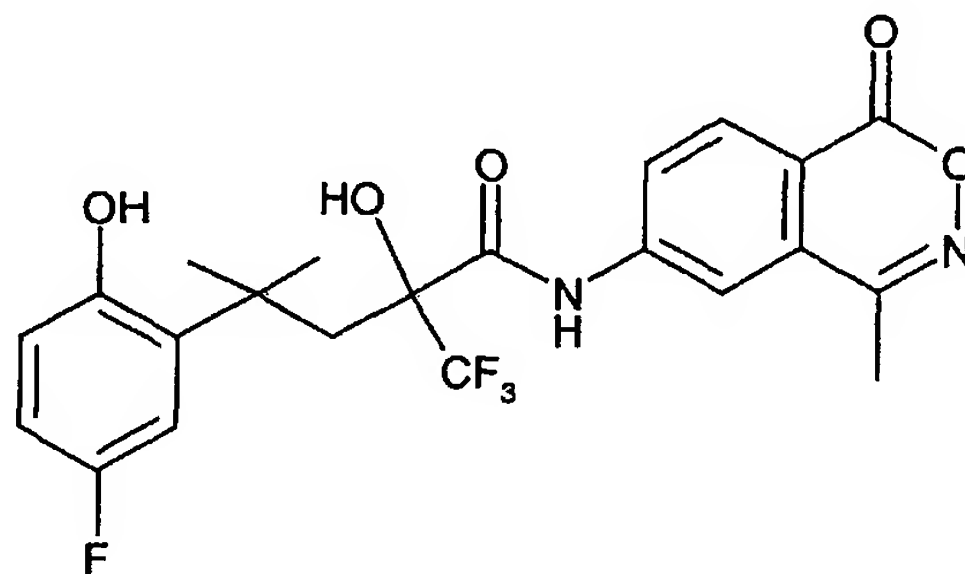
[0242] The GR/FP/TIF2 expanded binding pocket described herein can be employed to explain a significant amount of the SAR in the non-steroidal class of compounds for these receptors. Additional insight into the SAR of the steroidal class of glucocorticoids can also be obtained using these models derived from the GR/FP/TIF2 crystal structure.

[0243] The expanded binding pocket of GR can also be employed in the design of novel steroidal and non-steroidal glucocorticoids. For example, *de novo* design of these ligands can be carried out in the context of the crystal structure using both intuition, manual processing of compounds, or various *de novo* drug design programs such as LUDI™ (Accelrys Inc., San Diego, California, United States of America) and LEAPFROG™ (Tripos Inc., St. Louis, Missouri, United States of America), as discussed herein.

[0244] The GR/FP/TIF2 crystal structure (particularly the region comprising additional volume seen in the binding pocket of the GR/TIF2/FP structure, which contributes to the expanded binding pocket) can be further employed to construct quantitative structure-activity relationship (QSAR) models through the crystal structure or combination of the crystal structure, calculated molecular descriptors, or calculated properties of the crystal structure such as those derived from molecular mechanics (MM) calculations.

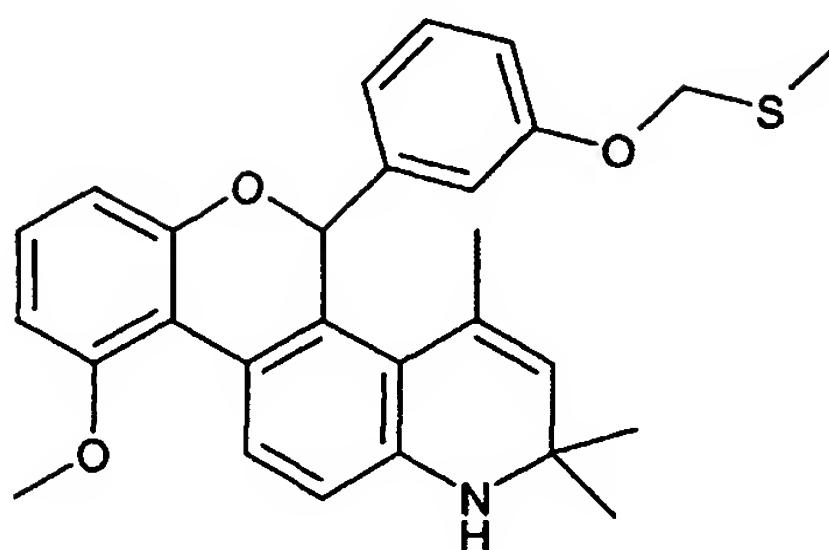
[0245] Thus, the region comprising additional volume seen in the binding pocket of the GR/TIF2/FP structure can be used in various capacities to explain the SAR of various binders of these proteins, to design *de novo* high affinity ligands, to predict the binding affinities or functional activity based on a QSAR model, or to electronically screen small to large collections of compounds at high-throughput.

[0246] As an example of the utility of the expanded binding pocket in modeling non-steroidal glucocorticoids, a docking model study was performed. The study involved the benzoxazin-1-one compound (Schering AG, Berlin, Germany; the compound is described in published PCT patent application WO 02/10143, incorporated herein by reference), which has the IUPAC name 4-(5-fluoro-2-hydroxyphenyl)-2-hydroxy-4-methyl-2-trifluoromethyl-pentanoic acid (4-methyl-1-oxo-1H-benzo[d][1,2]oxazine-6-yl)-amide and the chemical structure:



In one aspect of the present invention, this compound was modeled in the GR active site; the process and results of this modeling is presented hereinbelow in Example 6. Before the disclosure of the present invention, attempts to model this compound into the GR binding pocket were unsuccessful. Thus through the discovery of the expanded binding pocket, which forms another aspect of the present invention, a viable binding mode of this compound has been proposed.

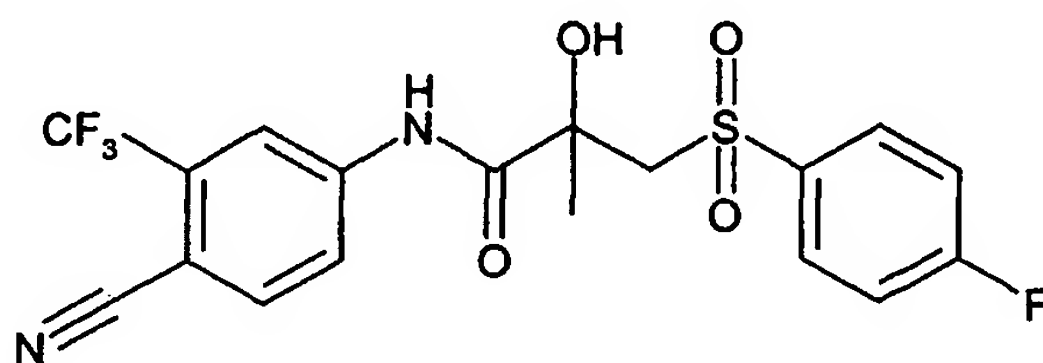
[0247] In a further example, the non-steroidal compound A-222977 was modeled in the GR active site (see Laboratory Example 9). A-222977 has the IUPAC name 10-methoxy-2,2,4-trimethyl-5-(3-methylsulfonylmethoxyphenyl)-2,5-dihydro-1H-6-oxa-1-azachrysene and the chemical structure:



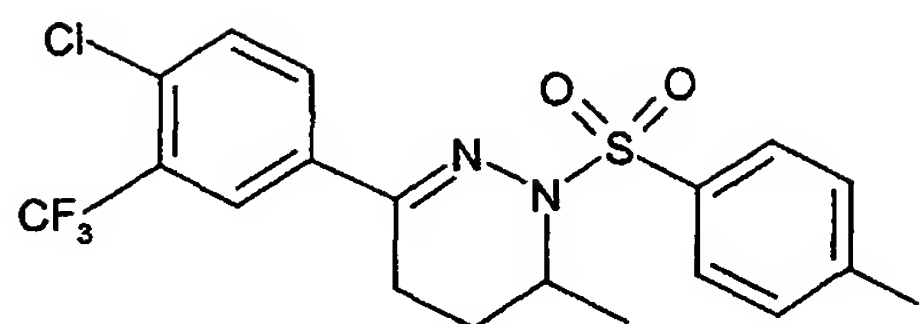
IX.C. Homology Modeling of Nuclear Receptors Using the GR/FP/TIF2 Crystal Structure

[0248] In yet another aspect of the present invention, the GR/FP structure disclosed herein can form a basis for generating homology models of other nuclear receptors. Homology modeling of a target protein generally involves the incremental substitution of amino acids of a related template protein in the attempt to produce a model of the target protein structure. This exercise assumes the template and target proteins to be related in their overall three-dimensional shape. This assumption is supported by other factors including similarity in primary amino acid sequence, receptor family membership, etc. A goal of creating a homology model can be, but need not be, to capture all of the detail usually found in a crystal structure. Preferably at least those essential portions of the protein's structure that are essential to describing its functional activity, small molecule binding properties, and other characteristics are considered. Therefore, to validate the utility of a homology model, it is preferable to infer from the model some explanation of experimentally observed data and/or information about the target protein, such as its binding affinities for various small molecules. Also, as further evidence relating a target protein's properties to its structure is acquired, it is possible to continue to refine various aspects of the homology model to account for this information. Thus, as more information is gathered and further experiments are conducted on the target protein, the homology model continues to improve and reflect the target protein's true functional nature.

[0249] For purposes of illustration, the generation of homology models of AR and PR based on a GR/FP/TIF2 structure of the present invention are discussed (see also Laboratory Examples 6-8). In the cases of AR and PR, crystal structures of these proteins have been determined previously for each of their respective natural steroidal ligands, dihydrotestosterone (DHT) (Sack et al., (2001) *Proc. Natl. Acad. Sci.* 98:4904-4909.) and progesterone (PG) (Williams & Sigler, (1998) *Nature* 393:392-396), and the steroidal compound R1881 (Matias et al., (2000) *J. Biol. Chem.* 275: 26164-26171). Although these crystal structures account for aspects of the steroidal structure activity relationships (SAR) among these receptors, the structures fail to account for the SAR of the non-steroidal compounds that are known to bind either or both AR and PR. For example, in the case of AR, bicalutamide (N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide) (U.S. Patent No. 4,636,505 and Tucker et al., (1988) *J. Med. Chem.* 31:954), a known, non-steroidal antagonist, binds AR with high-affinity, but this activity has not, and indeed cannot, be explained in the context of the AR crystal structures. Bicalutamide has the the IUPAC name *N*-(4-cyano-3-trifluoromethylphenyl)-3-(4-fluorobenzenesulfonyl)-2-hydroxy-2-methylpropionamide and the chemical structure:



Similarly, RWJ-60130 (U.S. Patent No. 5,684,151; Palmer et al., (2001) *J. Steroid. Biochem. Mol. Biol.* 75:33-42), a known, potent, non-steroidal agonist, binds PR with a high-affinity, but, as with AR and bicalutamide, its activity has not and cannot be explained in the context of the PR crystal structures. RWJ-60130 has the IUPAC name 3-(4-chloro-3-trifluoromethylphenyl)-1-(4-iodobenzenesulfonyl)-6-methyl-1,4,5,6-tetrahydropyridazine and the chemical structure:



In both cases, the inexplicability of the compounds' high affinity is related to the size of the compounds; these non-steroidal ligands are simply too large to fit in the ligand binding pockets as depicted in the AR and PR crystal structures.

[0250] With the solution of a GR/FP/TIF2 crystal structure and the appearance of an expanded binding pocket as provided by the present invention, construction of AR and PR (and other NR) homology models that explain the SAR of these large, potent binders became possible. Also, given the high sequence identity in the LBD of GR to AR (50%) and PR (54%) and receptor family similarity (as depicted hereinabove), a similar expanded binding pocket is expected to materialize in AR and PR under appropriate conditions. Thus, the construction of AR and PR homology models bound with bicalutamide and RWJ-60130, respectively, can be undertaken using the crystal structure of GR bound with FP and a TIF2 peptide.

[0251] It is noted that prior to the disclosure of the present invention, accurate AR, MR and PR homology and docking models could not be generated. Although structures for AR, MR and PR have been published, these structures do not account for the expanded binding pocket observed in the present GR/TIF2/FP structure. The presence of the expanded binding pocket is useful in explaining the observed binding of ligands to NRs. Models that do not include the expanded binding pocket cannot adequately explain observed binding modes. Therefore, models generated employing previous known NR structures that do not include the expanded binding pocket are incomplete and are not the best representation of the NR structures for which the models were generated. Moreover, models lacking the expanded binding pocket are not the best models to employ in the rational design of NR modulators.

[0252] Thus, in one embodiment, a data structure embodied in a computer-readable medium is provided. Preferably, the data structure comprises: a first data field containing data representing spatial coordinates of an NR LBD comprising an expanded binding pocket, wherein the first data field is derived by combining at least a part of a second data field with at least a part of a third data field, and wherein (a) the second data field contains data representing spatial coordinates of the atoms comprising a GR LBD comprising an expanded binding pocket in complex with a ligand; and (b) the third data field contains data representing spatial coordinates of the atoms comprising a NR LBD.

IX.C.1. Applications of NR Homology Models

[0253] The NR (and particularly AR, MR and PR) homology models described herein can be employed to explain a majority of the SAR in the non-steroidal class of compounds for these receptors. Additional insight into the SAR of the steroidal class of compounds for NRs, such as AR and PR can also be obtained using these models.

[0254] These models can be employed in the design of novel steroidal and non-steroidal ligands for NRs (e.g. AR, MR and PR). For example, *de novo* design of NR ligands can be carried out in the context of these homology models using both intuition, manual processing of compounds, or various *de novo* drug design programs such as LUDI™ (Accelrys Inc., San Diego, California United States of America) and LEAPFROG™ (Tripos Inc., St. Louis, Missouri, United States of America).

[0255] The models can be used to construct quantitative structure-activity relationship (QSAR) models solely through the homology models or through the combination of the models, calculated molecular descriptors, or calculated properties of the homology models such as those derived from molecular mechanics (MM) calculations.

[0256] Thus, the homology models of the present invention can be employed in various capacities to explain the SAR of various binders of these proteins, *de novo* design of high affinity ligands, predict the binding affinities or functional activity based on a QSAR model, or electronically high-throughput screen small to large collections of compounds.

IX.C.2. Method of Forming a Homology Model of an NR

[0257] In one aspect of the present invention a method of forming a homology model of an NR is disclosed. In a preferred embodiment, the method comprises: (a) providing a template amino acid sequence comprising a GR complex comprising a large pocket volume as disclosed herein; (b) providing a target NR amino acid sequence; (c) aligning the target sequence and the template sequence to form a homology model. Preferably, the template amino acid comprises the LBD of GR α in complex with a co-activator peptide and fluticasone propionate.

[0258] This preferred method is best illustrated by way of specific example, namely the construction of an AR ho-

mology model. Those of ordinary skill in the art will appreciate that although the method is presented in the context of generating an AR homology model, the method can be employed *mutatis mutandis* to generate homology models for any NR.

[0259] In the formulation of an AR homology model based on the GR/FP/TIF2 structure of the present invention, sequence alignments of the AR and GR LBDs can be initially obtained using the alignment algorithm implemented in MVP (Lambert, (1997) in Practical Application of Computer-Aided Drug Design (Charifson, ed.), Marcel Dekker, New York, New York, United States of America, pp 243-303). Target NRs that can be characterized in terms of atomic coordinates are especially preferred, due to the relative ease of manipulation. In this specific example of the preferred method, the GR LBD, which is more preferably derived from the GR/FP/TIF2 structure disclosed herein, is the template amino acid sequence. The AR amino acid sequence is the target NR amino acid sequence in this example.

[0260] After three-dimensional alignment and coordinate translation of the GR/FP crystal structure into a standard orientation using MVP, a desired subunit can be selected for use in the homology model. For example, the second subunit of the GR/FP/TIF2 structure can be selected when constructing an AR homology model. Throughout the process of building a homology model, the Homology package in the INSIGHTII program (Accelrys Inc., San Diego, California, United States of America) or a similar computer software package can be used to visualize the proteins, extract the LBD sequences, manually align the sequences, transform the amino acid residues, manually manipulate the amino acid sidechain conformers, and export the three-dimensional coordinates in appropriate file formats.

[0261] A desired subunit (e.g. the second subunit of the GR/FP/TIF2 structure) can be loaded into the display area of INSIGHTII along with the target NR structure (e.g. the AR/DHT structure) for comparison purposes. Following any desired comparison, the Homology package can be used to extract the template and target (e.g. the GR and AR, respectively) primary amino acid sequences. The sequences are preferably extracted from crystal structure coordinate files, although a target NR amino acid sequence can also be manually built and manipulated. If desired, the sequences can then be manually aligned using Homology and by comparison with those alignments obtained using the MVP program.

[0262] Next, a transformation of the amino acid residues can be performed. A desired transformation can be carried out and initial three-dimensional coordinates of the NR homology model can be assigned using the AssignCoords method in the Homology modeling package or another suitable software package. When assigning coordinates to an NR in a homology model, corresponding residues in a template sequence can be employed. For example, when assigning the coordinates of residues I672-K883 in the AR homology model, the corresponding coordinates of residues T531-D742 in the GR/FP crystal structure were used. Additionally, when assigning the coordinates of residues M886-H917 in the AR homology model, the corresponding coordinates of residues K744-H775 in the GR/FP/TIF2 crystal structure were used. Finally, when assigning the coordinates of residues S884-H885 in the AR homology model, the corresponding coordinates from the AR/DHT crystal structure were used.

[0263] Following transformation and assignment of coordinates in an NR homology model, it might be desirable to manually manipulate the homology model. Desired manual modifications of amino acid side chain conformers can be carried out after comparing the conformations of corresponding residues in the initial homology model and the crystal structure of the target sequence.

[0264] Table 4 presents the three-dimensional coordinates of AR in complex with bicalutamide obtained from homology modeling of the crystal structure coordinates of GR α in complex with FP, as derived from the disclosed method. Table 5 presents the three-dimensional coordinates of PR in Complex with RWJ-60130 obtained from homology modeling of the crystal structure coordinates of GR α in complex with FP.

IX.C.3. Method of Modeling the Interaction Between an NR and a Ligand

[0265] In another aspect of the present invention, a method of modeling an interaction between an NR and a non-steroid ligand is provided. In a preferred embodiment, the method comprises: (a) providing a homology model of a target NR generated using a GR complex that comprises an expanded binding pocket as disclosed herein; (b) providing coordinates of a non-steroid ligand; (c) docking the non-steroid ligand with homology model to form a NR/ligand model; and (d) optimizing the geometry of the NR/ligand model, whereby an interaction between an NR and a non-steroid ligand is modeled.

[0266] As noted, a GR complex that comprises an expanded binding pocket as disclosed herein can be employed to model an interaction between an NR and a ligand. In the following section, a preferred method of modeling an interaction between an NR and a ligand is presented by way of specific example, namely modeling an interaction between PR and the ligand RWJ-60130. Those of ordinary skill in the art will appreciate that although the method is presented in the context of modeling an interaction between a PR and RWJ-60130, the method can be employed *mutatis mutandis* to model an interaction between any NR and a ligand.

[0267] First, a homology model can be constructed. Construction of such a model can be achieved by employing the method disclosed in detail in section IX.C.2. hereinabove. Although the precise steps of forming a homology model

for a PR using the GR/FP/TIF2 structure that forms an aspect of the present invention are not presented here, preferred steps mirror, *mutatis mutandis*, those presented hereinabove in the formation of an AR homology model. The following discussion assumes the preparation of a PR homology model.

[0268] Continuing with the preferred method, initial coordinates for a non-steroid ligand are provided. Coordinates for a non-steroid ligand can be generated using any suitable software package; the software package CONCORD v4.0.4 (Tripos Inc., St. Louis, Missouri, United States of America) is especially preferred. In the present specific example, initial coordinates of the PR ligand RWJ-60130 are generated using CONCORD v4.0.4.

[0269] Next, any desired ligand conformers are generated. These ligand conformers can be generated using software adapted for that purpose. Preferred software includes the GROW algorithm available in MVP and optimized using the CVFF module, as implemented in MVP. In the context of the present PR example, a number of conformers of the initial RWJ-60130 geometry are generated.

[0270] Subsequently, the ligand conformers are docked into the homology model. This operation can be performed using, for example, the DOCK module of INSIGHTII. Each generated conformer can be automatically or manually docked into the homology model and evaluated for goodness of fit. The evaluation can comprise a computational analysis of the ligand-NR structure or it can be a simple visual inspection of the structure. The best fitting conformer is taken as representative of the conformation the ligand takes when it binds the NR. Continuing with the PR/RWJ-60130 complex example, each of the resulting conformers are hand-docked into the initial PR homology model and the best-fitting conformer is selected as the proposed binding conformation of RWJ-60130.

[0271] After docking of the best-fitting conformer into the NR, the complex is modified as desired, for example to correct residue numbering. MVP can be employed to perform any desired modifications. With reference to the example of the PR/RWJ-60130 complex, the complex is exported from INSIGHTII in the identical coordinate reference frame as the GR/FP/TIF2 crystal structure. MVP and the sequence alignments of GR and PR are employed to correct the residue numbering of the initial PR model.

[0272] Finally, optimization of the geometry of the NR/ligand model is performed. Again, suitable software can be employed to perform the optimization. Although any software can be employed, the CVFF software package of MVP is preferred for carrying out the optimization operation. Desirable settings and conditions for the optimization will be known to those of ordinary skill in the art upon consideration of the present disclosure. By way of specific example, geometry optimization of the PR/RWJ-60130 homology model complex is carried out using CVFF as implemented in MVP, as noted above. All atoms in the complex are fixed in space except for those atoms contained in RWJ-60130 and the initial PR model that were within a desired distance constraint, for example within 6 angstroms of any atom in RWJ-60130. The CVFF energy terms are calculated using only those atoms within desired distance constraint of the ligand, for example within 16 angstroms of (and including) RWJ-60130. Geometry optimization of the protein-ligand complex is preferably carried out using the conjugate gradient method as implemented in MVP and with a convergence criteria of a 0.1 change in the gradient.

[0273] Table 6 presents a subset of the three-dimensional coordinates of GR in complex with the Benzoxazin-1-one obtained from modeling of the crystal structure of GR α in complex with FP. Table 7 presents a subset of the three-dimensional coordinates of GR α in complex with A-222977 obtained from modeling of the crystal structure of GR α in complex with FP.

IX.C.4. Method of Designing a Non-steroid Modulator of an NR Using a Homology Model

[0274] In yet another embodiment of the present invention, a method of designing a non-steroid modulator of an NR using a homology model is disclosed. In a preferred embodiment, the method comprises: (a) modeling an interaction between an NR and a non-steroid ligand using the structure of a GR complex comprising a large pocket volume; (b) evaluating the interaction between the NR and the non-steroid ligand to determine a first binding efficiency; (c) modifying the structure of the non-steroid ligand to form a modified ligand; (d) modeling an interaction between the modified ligand and the NR; (e) evaluating the interaction between the NR and the modified ligand to determine a second binding efficiency; and (f) repeating steps (c)-(e) a desired number of times if the second binding efficiency is less than the first binding efficiency. The disclosed method can be applied to any NR.

[0275] In one embodiment, an interaction between an NR and a non-steroid ligand is modeled using the structure of a GR α LBD in complex with TIF2 and fluticasone propionate, an aspect of the present invention. Such an interaction can be modeled using the steps disclosed hereinabove in section IX.C.3.

[0276] Next, the interaction between the NR and the non-steroid ligand is evaluated in order to determine a first binding efficiency. The evaluation can be quantitative or qualitative. When a quantitative comparison is desired, software programs can be employed to calculate various binding parameters, which can be subsequently analyzed to arrive at one or more parameters that described aspects of binding efficiency.

[0277] Following an assessment of a first binding efficiency, the structure of the non-steroid ligand is modified to form a modified ligand. Such modification can include altering one or more properties of the ligand predicted to enhance

binding efficiency of the ligand to the NR. The modification(s) is preferably performed using a suitable software package. Modules of software packages INSIGHTII and/or MVP can be employed to accomplish any desired modification(s). The modification(s) can take any of a variety of forms, for example functional groups can be replaced and bond angles can be altered.

5 [0278] Then, an interaction between the modified ligand and the NR can be modeled. Again, the interaction can be modeled using the steps disclosed hereinabove and in section IX.C.3.

[0279] Finally, the interaction between the NR and the modified ligand is evaluated to determine a second binding efficiency. As described above, software programs can be employed to calculate various binding parameters and binding parameters. A quantitative assessment of a second binding efficiency is preferred.

10 [0280] Lastly, the above steps are repeated a desired number of times if the second binding efficiency is less than the first binding efficiency. By performing multiple iterations of the above method, a non-steroid ligand can be designed using a GR complex comprising a large pocket volume in accordance with the present invention.

IX.D. Method of Screening for Chemical and Biological Modulators of the Biological Activity of an NR

15 [0281] A candidate substance identified according to a screening assay of the present invention has an ability to modulate the biological activity of an NR or an NR LBD polypeptide. In a preferred embodiment, such a candidate compound can have utility in the treatment of disorders and/or conditions and/or biological events associated with the biological activity of an NR or an NR LBD polypeptide, including transcription modulation.

20 [0282] In a cell-free system, the method preferably comprises the steps of establishing a control system comprising a GR α polypeptide and a ligand which is capable of binding to the polypeptide; establishing a test system comprising a GR α polypeptide, the ligand, and a candidate compound; and determining whether the candidate compound modulates the activity of the polypeptide by comparison of the test and control systems. A representative ligand can comprise fluticasone propionate or other small molecule, and in this embodiment, the biological activity or property screened can include binding affinity or transcription regulation. The GR α polypeptide can be in soluble or crystalline form.

25 [0283] In another embodiment of the invention, a soluble or a crystalline form of a GR α polypeptide or a catalytic or immunogenic fragment or oligopeptide thereof, can be used for screening libraries of compounds in any of a variety of drug screening techniques. The fragment employed in such a screening can be affixed to a solid support. The formation of binding complexes, between a soluble or a crystalline GR α polypeptide and the agent being tested, will be detected. In a preferred embodiment, the soluble or crystalline GR α polypeptide has an amino acid sequence of any of SEQ ID NOs: 2 and 4. When a GR α LBD polypeptide is employed, a preferred embodiment includes a soluble or a crystalline GR α polypeptide having the amino acid sequence of any of SEQ ID NOs: 6 and 8.

30 [0284] Another technique for drug screening which can be used provides for high throughput screening of compounds having suitable binding affinity to the protein of interest as described in published PCT application WO 84/03564, herein incorporated by reference. In this method, as applied to a soluble or crystalline polypeptide of the present invention, large numbers of different small test compounds are synthesized on a solid substrate, such as plastic pins or some other surface. The test compounds are reacted with the soluble or crystalline polypeptide, or fragments thereof. Bound polypeptide is then detected by methods known to those of skill in the art. The soluble or crystalline polypeptide can also be placed directly onto plates for use in the aforementioned drug screening techniques.

40 [0285] In yet another embodiment, a method of screening for a modulator of an NR or an NR LBD polypeptide comprises: providing a library of test samples; contacting a soluble or a crystalline form of an NR or a soluble or crystalline form of an NR LBD polypeptide with each test sample; detecting an interaction between a test sample and a soluble or a crystalline form of an NR or a soluble or a crystalline form of an NR LBD polypeptide; identifying a test sample that interacts with a soluble or a crystalline form of an NR or a soluble or a crystalline form of an NR LBD polypeptide; and isolating a test sample that interacts with a soluble or a crystalline form of an NR or a soluble or a crystalline form of an NR LBD polypeptide.

45 [0286] In each of the foregoing embodiments, an interaction can be detected spectrophotometrically, radiologically, colorimetrically or immunologically. An interaction between a soluble or a crystalline form of an NR or a soluble or a crystalline form of an NR LBD polypeptide and a test sample can also be quantified using methodology known to those of skill in the art.

50 [0287] In accordance with the present invention there is also provided a rapid and high throughput screening method that relies on the methods described above. This screening method comprises separately contacting each of a plurality of substantially identical samples with a soluble or a crystalline form of an NR or a soluble or a crystalline form of an NR LBD and detecting a resulting binding complex. In such a screening method the plurality of samples preferably comprises more than about 10^4 samples, or more preferably comprises more than about 5×10^4 samples.

55 [0288] In another embodiment, a method for identifying a substance that modulates GR LBD function is also provided. In a preferred embodiment, the method comprises: (a) isolating a GR polypeptide of the present invention; (b) exposing the isolated GR polypeptide to a plurality of substances; (c) assaying binding of a substance to the isolated GR polypep-

tion; and (d) selecting a substance that demonstrates specific binding to the isolated GR LBD polypeptide. By the term "exposing the GR polypeptide to a plurality of substances", it is meant both in pools and as multiple samples of "discrete" pure substances.

5 IX.E. Method of Identifying Compounds Which Inhibit Ligand Binding

[0289] In one aspect of the present invention, an assay method for identifying a compound that inhibits binding of a ligand to an NR polypeptide is disclosed. A ligand, such as fluticasone propionate (which associates with at least GR), can be employed in the assay method as the ligand against which the inhibition by a test compound is gauged. In the following discussion of Section IX.E., it will be understood that although GR is used as an example, the method is equally applicable to any of NR polypeptide. The method comprises (a) incubating a GR polypeptide with a ligand in the presence of a test inhibitor compound; (b) determining an amount of ligand that is bound to the GR polypeptide, wherein decreased binding of ligand to the GR polypeptide in the presence of the test inhibitor compound relative to binding in the absence of the test inhibitor compound is indicative of inhibition; and (c) identifying the test compound as an inhibitor of ligand binding if decreased ligand binding is observed. Preferably, the ligand is fluticasone propionate. [0290] In another aspect of the present invention, the disclosed assay method can be used in the structural refinement of candidate GR inhibitors. For example, multiple rounds of optimization can be followed by gradual structural changes in a strategy of inhibitor design. A strategy such as this is facilitated by the disclosure of the atomic coordinates of a GR complex in accordance with the present invention.

20 X. Design, Preparation and Structural Analysis of Additional NR Polypeptides and NR LBD Mutants and Structural Equivalents

[0291] The present invention provides for the generation of NR polypeptides and NR (preferably GR α and GR α LBD mutants), and the ability to solve the crystal structures of those that crystallize. Thus, an aspect of the present invention involves the use of both targeted and random mutagenesis of the GR gene for the production of a recombinant protein with improved or desired characteristics for the purpose of crystallization, characterization of biologically relevant protein-protein interactions, and compound screening assays, or for the production of a recombinant protein having another desirable characteristic(s). Polypeptide products produced by the methods of the present invention are also disclosed herein.

[0292] The structure coordinates of a NR LBD provided in accordance with the present invention also facilitate the identification of related proteins or enzymes analogous to GR α in function, structure or both, (for example, a GR β) which can lead to novel therapeutic modes for treating or preventing a range of disease states. More particularly, through the provision of the mutagenesis approaches as well as the three-dimensional structure of a GR α LBD disclosed herein, desirable sites for mutation are identified.

X.A. Design and Preparation of Sterically Similar Compounds

[0293] A further aspect of the present invention is that sterically similar compounds can be formulated to mimic the key portions of an NR LBD structure. Such compounds are functional equivalents. The generation of a structural functional equivalent can be achieved by the techniques of modeling and chemical design known to those of skill in the art and described herein. Modeling and chemical design of NR and NR LBD structural equivalents can be based on the structure coordinates of a crystalline GR α LBD polypeptide of the present invention. It will be understood that all such sterically similar constructs fall within the scope of the present invention.

X.B. Design and Preparation of NR Polypeptides

[0294] The generation of chimeric GR polypeptides is also an aspect of the present invention. Such a chimeric polypeptide can comprise an NR LBD polypeptide or a portion of an NR LBD, (e.g. a GR α LBD) that is fused to a candidate polypeptide or a suitable region of the candidate polypeptide, for example GR β . Throughout the present disclosure it is intended that the term "mutant" encompass not only mutants of an NR LBD polypeptide but chimeric proteins generated using an NR LBD as well. It is thus intended that the following discussion of mutant NR LBDs apply *mutatis mutandis* to chimeric NR polypeptides and NR LBD polypeptides and to structural equivalents thereof.

[0295] In accordance with the present invention, a mutation can be directed to a particular site or combination of sites of a wild-type NR LBD. For example, an accessory binding site or the binding pocket can be chosen for mutagenesis. Similarly, a residue having a location on, at or near the surface of the polypeptide can be replaced, resulting in an altered surface charge of one or more charge units, as compared to the wild-type NR and NR LBDs. Alternatively, an amino acid residue in an NR or an NR LBD can be chosen for replacement based on its hydrophilic or hydrophobic

characteristics.

[0296] Such mutants can be characterized by any one of several different properties, i.e. a "desired" or "predetermined" characteristic as compared with the wild type NR LBD. For example, such mutants can have an altered surface charge of one or more charge units, or can have an increase in overall stability. Other mutants can have altered substrate specificity in comparison with, or a higher specific activity than, a wild-type NR or an NR LBD.

[0297] NR and NR LBD mutants of the present invention can be generated in a number of ways. For example, the wild-type sequence of an NR or an NR LBD can be mutated at those sites identified using this invention as desirable for mutation, by means of oligonucleotide-directed mutagenesis or other conventional methods, such as deletion. Alternatively, mutants of an NR or an NR LBD can be generated by the site-specific replacement of a particular amino acid with an unnaturally occurring amino acid. In addition, NR or NR LBD mutants can be generated through replacement of an amino acid residue, for example, a particular cysteine or methionine residue, with selenocysteine or selenomethionine. This can be achieved by growing a host organism capable of expressing either the wild-type or mutant polypeptide on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

[0298] As disclosed in the Examples presented below, mutations can be introduced into a DNA sequence coding for a NR or an NR LBD using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired mutation sites. Mutations can be generated in the full-length DNA sequence of a NR or an NR LBD or in any sequence coding for polypeptide fragments of an NR or an NR LBD.

[0299] According to the present invention, a mutated NR or NR LBD DNA sequence produced by the methods described above, or any alternative methods known in the art, can be expressed using an expression vector. An expression vector, as is well known to those of skill in the art, typically includes elements that permit autonomous replication in a host cell independent of the host genome, and one or more phenotypic markers for selection purposes. Either prior to or after insertion of the DNA sequences surrounding the desired NR or NR LBD mutant coding sequence, an expression vector also will include control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes and a signal for termination. In some embodiments, where secretion of the produced mutant is desired, nucleotides encoding a "signal sequence" can be inserted prior to an NR or an NR LBD mutant coding sequence. For expression under the direction of the control sequences, a desired DNA sequence must be operatively linked to the control sequences; that is, the sequence must have an appropriate start signal in front of the DNA sequence encoding the NR or NR LBD mutant, and the correct reading frame to permit expression of that sequence under the control of the control sequences and production of the desired product encoded by that NR or NR LBD sequence must be maintained.

[0300] After a review of the disclosure of the present invention presented herein, any of a wide variety of well-known available expression vectors can be useful to express a mutated coding sequence of this invention. These include for example, vectors consisting of segments of chromosomal, non-chromosomal and synthetic DNA sequences, such as various known derivatives of SV40, known bacterial plasmids, e.g., plasmids from *E. coli* including col E1, pCR1, pBR322, pMB9 and their derivatives, wider host range plasmids, e.g., RP4, phage DNAs, e.g., the numerous derivatives of phage λ , e.g., NM 989, and other DNA phages, e.g., M13 and filamentous single stranded DNA phages, yeast plasmids and vectors derived from combinations of plasmids and phage DNAs, such as plasmids which have been modified to employ phage DNA or other expression control sequences. In the preferred embodiments of this invention, vectors amenable to expression in a pET-based expression system are employed. The pET expression system is available from Novagen/Invitrogen, Inc. of Carlsbad, California. Expression and screening of a polypeptide of the present invention in bacteria, preferably *E. coli*, is a preferred aspect of the present invention.

[0301] In addition, any of a wide variety of expression control sequences--sequences that control the expression of a DNA sequence when operatively linked to it--can be used in these vectors to express the mutated DNA sequences according to this invention. Such useful expression control sequences, include, for example, the early and late promoters of SV40 for animal cells, the lac system, the trp system the TAC or TRC system, the major operator and promoter regions of phage λ , the control regions of fd coat protein, all for *E. coli*, the promoter for 3-phosphoglycerate kinase or other glycolytic enzymes, the promoters of acid phosphatase, e.g., Pho5, the promoters of the yeast α -mating factors for yeast, and other sequences known to control the expression of genes of prokaryotic or eukaryotic cells or their viruses, and various combinations thereof.

[0302] A wide variety of hosts are also useful for producing mutated NR, SR or GR and NR, SR or GR LBD polypeptides according to this invention. These hosts include, for example, bacteria, such as *E. coli*, *Bacillus* and *Streptomyces*, fungi, such as yeasts, and animal cells, such as CHO and COS-1 cells, plant cells, insect cells, such as SF9 cells, and transgenic host cells. Expression and screening of a polypeptide of the present invention in bacteria, preferably *E. coli*, is a preferred aspect of the present invention.

[0303] It should be understood that not all expression vectors and expression systems function in the same way to express mutated DNA sequences of this invention, and to produce modified NR, SR or GR and NR, SR or GR LBD polypeptides or NR, SR or GR or NR, SR or GR LBD mutants. Neither do all hosts function equally well with the same

expression system. One of skill in the art can, however, make a selection among these vectors, expression control sequences and hosts without undue experimentation and without departing from the scope of this invention. For example, an important consideration in selecting a vector will be the ability of the vector to replicate in a given host. The copy number of the vector, the ability to control that copy number, and the expression of any other proteins encoded

by the vector, such as antibiotic markers, should also be considered. These include, [0304] In selecting an expression control sequence, a variety of factors should also be considered. These include, for example, the relative strength of the system, its controllability and its compatibility with the DNA sequence encoding a modified NR or NR LBD polypeptide of this invention, with particular regard to the formation of potential secondary and tertiary structures.

[0305] Hosts should be selected by consideration of their compatibility with the chosen vector, the toxicity of a modified polypeptide to them, their ability to express mature products, their ability to fold proteins correctly, their fermentation requirements, the ease of purification of a modified GR or GR LBD and safety. Within these parameters, one of skill in the art can select various vector/expression control system/host combinations that will produce useful amounts of a mutant polypeptide. A mutant polypeptide produced in these systems can be purified, for example, via the approaches disclosed in the Laboratory Examples.

[0306] Once a mutation(s) has been generated in the desired location, such as an active site or dimerization site, the mutants can be tested for any one of several properties of interest, i.e. "desired" or "predetermined" positions. For example, mutants can be screened for an altered charge at physiological pH. This property can be determined by measuring the mutant polypeptide isoelectric point (pI) and comparing the observed value with that of the wild-type parent. Isoelectric point can be measured by gel-electrophoresis according to the method of Wellner (Wellner, (1971) *Anal. Chem.* 43:597). A mutant polypeptide containing a replacement amino acid located at the surface of the enzyme, as provided by the structural information of this invention, can lead to an altered surface charge and an altered pI.

X.C. Generation of an NR or NR LBD Mutants

[0307] In another aspect of the present invention, a unique NR or NR LBD polypeptide is generated. Such a mutant can facilitate purification and the study of the structure and the ligand-binding abilities of a NR polypeptide. Thus, an aspect of the present invention involves the use of both targeted and random mutagenesis of the GR gene for the production of a recombinant protein with improved solution characteristics for the purpose of crystallization, characterization of biologically relevant protein-protein interactions, and compound screening assays, or for the production of a recombinant polypeptide having other characteristics of interest. Expression of the polypeptide in bacteria, preferably *E. coli*, is also an aspect of the present invention.

[0308] In one embodiment, targeted mutagenesis was performed using a sequence alignment of several nuclear receptors, primarily steroid receptors. Several residues that were hydrophobic in GR and hydrophilic in other receptors were chosen for mutagenesis. Most of these residues were predicted to be solvent exposed hydrophobic residues in GR. Therefore, mutations were made to change these hydrophobic residues to hydrophilic in attempt to improve the solubility and stability of *E.coli*-expressed GR LBD.

[0309] Random mutagenesis can be performed on residues where a significant difference, hydrophobic versus hydrophilic, is observed between GR and other steroid receptors based on sequence alignment. Such positions can be randomized by oligo-directed or cassette mutagenesis. A GR LBD protein library can be sorted by an appropriate display system to select mutants with improved solution properties. Residues in GR that meet the criteria for such an approach include: V538, V552, W557, F602, L636, Y648, Y660, L685, M691, V702, W712, L733, and Y764. In addition, residues predicted to neighbor these positions can also be randomized.

[0310] A method of modifying a test NR polypeptide is thus disclosed. The method can comprise: providing a test NR polypeptide sequence having a characteristic that is targeted for modification; aligning the test NR polypeptide sequence with at least one reference NR polypeptide sequence for which an X-ray structure is available, wherein the at least one reference NR polypeptide sequence has a characteristic that is desired for the test NR polypeptide; building a three-dimensional model for the test NR polypeptide using the three-dimensional coordinates of the X-ray structure (s) of the at least one reference polypeptide and its sequence alignment with the test NR polypeptide sequence; examining the three-dimensional model of the test NR polypeptide for differences with the at least one reference polypeptide that are associated with the desired characteristic; and mutating at least one amino acid residue in the test NR polypeptide sequence located at a difference identified above to a residue associated with the desired characteristic, whereby the test NR polypeptide is modified. By the term "associated with a desired characteristic" it is meant that a residue is found in the reference polypeptide at a point of difference wherein the difference provides a desired characteristic or phenotype in the reference polypeptide.

[0311] A method of altering the solubility of a test NR polypeptide is also disclosed in accordance with the present invention. In a preferred embodiment, the method comprises: (a) providing a reference NR polypeptide sequence and a test NR polypeptide sequence; (b) comparing the reference NR polypeptide sequence and the test NR polypeptide

sequence to identify one or more residues in the test NR sequence that are more or less hydrophilic than a corresponding residue in the reference NR polypeptide sequence; and (c) mutating the residue in the test NR polypeptide sequence identified in step (b) to a residue having a different hydrophilicity, whereby the solubility of the test NR polypeptide is altered.

5 [0312] By the term "altering" it is meant any change in the solubility of the test NR polypeptide, including preferably a change to make the polypeptide more soluble. Such approaches to obtain soluble proteins for crystallization studies have been successfully demonstrated in the case of HIV integration intergrase and the human leptin cytokine. See Dyda et al., (1994) *Science* 266:1981-86; and Zhang et al., (1997) *Nature* 387:206-209.

10 [0313] Typically, such a change involves substituting a residue that is more hydrophilic than the wild type residue. Hydrophobicity and hydrophilicity criteria and comparison information are set forth herein below. Optionally, the reference NR polypeptide sequence is an AR or a PR sequence, and the test polypeptide sequence is a GR polypeptide sequence. Alternatively, the reference polypeptide sequence is a crystalline GR LBD. The comparing of step (b) is preferably by sequence alignment. More preferably, the screening is carried out in bacteria, even more preferably, in *E. coli*.

15 [0314] A method for modifying a test NR polypeptide to alter and preferably improve the solubility, stability in solution and other solution behavior, to alter and preferably improve the folding and stability of the folded structure, and to alter and preferably improve the ability to form ordered crystals is also provided in accordance with the present invention. The aforementioned characteristics are representative "desired" or "predetermined characteristics or phenotypes.

20 [0315] In a preferred embodiment, the method comprises: (a) providing a test NR polypeptide sequence for which the solubility, stability in solution, other solution behavior, tendency to fold properly, ability to form ordered crystals, or combination thereof is different from that desired; (b) aligning the test NR polypeptide sequence with the sequences of other reference NR polypeptides for which the X-ray structure is available and for which the solution properties, folding behavior and crystallization properties are closer to those desired; (c) building a three-dimensional model for the test NR polypeptide using the three-dimensional coordinates of the X-ray structure(s) of one or more of the reference polypeptides and their sequence alignment with the test NR polypeptide sequence; (d) optionally, optimizing the side-chain conformations in the three-dimensional model by generating many alternative side-chain conformations, refining by energy minimization, and selecting side-chain conformations with lower energy; (e) examining the three-dimensional model for the test NR graphically for lipophilic side-chains that are exposed to solvent, for clusters of two or more lipophilic side-chains exposed to solvent, for lipophilic pockets and clefts on the surface of the protein model, and in particular for sites on the surface of the protein model that are more lipophilic than the corresponding sites on the structure(s) of the reference NR polypeptide(s); (f) for each residue identified in step (e), mutating the amino acid to an amino acid with different hydrophilicity, and usually to a more hydrophilic amino acid, whereby the exposed lipophilic sites are reduced, and the solution properties improved; (g) examining the three-dimensional model graphically at each site where the amino acid in the test NR polypeptide is different from the amino acid at the corresponding position in the reference NR polypeptide, and checking whether the amino acid in the test NR polypeptide makes favorable interactions with the atoms that lie around it in the three-dimensional model, considering the side-chain conformations predicted in steps (c) and, optionally step (d), as well as likely alternative conformations of the side-chains, and also considering the possible presence of water molecules (for this analysis, an amino acid is considered to make "favorable interactions with the atoms that lie around it" if these interactions are more favorable than the interactions that would be obtained if it was replaced by any of the 19 other naturally-occurring amino acids); (h) for each residue identified in step (g) as not making favorable interactions with the atoms that lie around it, mutating the residue to another amino acid that could make better interactions with the atoms that lie around it, thereby promoting the tendency for the test NR polypeptide to fold into a stable structure with improved solution properties, less tendency to unfold, and greater tendency to form ordered crystals; (i) examining the three-dimensional model graphically at each residue position where the amino acid in the test NR polypeptide is different from the amino acid at the corresponding position in the reference NR polypeptide, and checking whether the steric packing, hydrogen bonding and other energetic interactions could be improved by mutating that residue or any one or more of the surrounding residues lying within 8 angstroms in the three-dimensional model; (j) for each residue position identified in step (i) as potentially allowing an improvement in the packing, hydrogen bonding and energetic interactions, mutating those residues individually or in combination to residues that could improve the packing, hydrogen bonding and energetic interactions, thereby promoting the tendency for the test NR polypeptide to fold into a stable structure with improved solution properties, less tendency to unfold, and greater tendency to form ordered crystals.

55 [0316] By the term "graphically" it is meant through the use of computer aided graphics, such by the use of a software package disclosed herein above. Optionally, in this embodiment, the reference NR polypeptide is AR, or PR, when the test NR polypeptide is GR α . Alternatively, the reference NR polypeptide is GR α , and the test NR polypeptide is preferably GR β , AR, PR or MR.

[0317] An isolated GR polypeptide comprising a mutation in a ligand binding domain, wherein the mutation alters the solubility of the ligand binding domain, is also disclosed. An isolated GR polypeptide, or functional portion thereof,

having one or more mutations comprising a substitution of a hydrophobic amino acid residue by a hydrophilic amino acid residue in a ligand binding domain is also disclosed. Preferably, in each case, the mutation can be at a residue selected from the group consisting of V552, W557, F602, L636, Y648, W712, L741, L535, V538, C638, M691, V702, Y648, Y660, L685, M691, V702, W712, L733, Y764 and combinations thereof. More preferably, the mutation is selected from the group consisting of V552K, W557S, F602S, F602D, F602E, F602Y, F602T, F602N, F602C, L636E, Y648Q, W712S, L741R, L535T, V538S, C638S, M691T, V702T, W712T and combinations thereof. Even more preferably, the mutation is made by targeted point or randomizing mutagenesis. Hydrophobicity and hydrophilicity criteria and comparison information are set forth herein below.

[0318] As discussed above, the GR α gene can be translated from its mRNA by alternative initiation from an internal ATG codon (Yudt & Cidlowski, (2001) *Molec. Endocrinol.* 15: 1093-1103). This codon codes for methionine at position 27 and translation from this position produces a slightly smaller protein. These two isoforms, translated from the same gene, are referred to as GR-A and GR-B. It has been shown in a cellular system that the shorter GR-B form is more effective in initiating transcription from a GRE compared to GR-A. Additionally, another form of GR, called GR β is produced by an alternative splicing event. The GR β protein differs from GR α at the very C-terminus, where the final 50 amino acids are replaced with a 15 amino acid segment. These two isoforms are 100% identical up to amino acid 727. No sequence similarity exists between GR α and GR β at the C-terminus beyond position 727. GR β has been shown to be a dominant negative regulator of GR α -mediated gene transcription (Oakley, et al., (1996) *J. Biol. Chem.* 271: 9550-9559). It has been suggested that some of the tissue specific effects observed with glucocorticoid treatment may in part be due to the presence of varying amounts of isoform in certain cell-types. This method is also applicable to any other subfamily so organized. Thus, while the amino acid residue numbers referenced above pertain to GR-A, the polypeptides of the present invention also have a mutation at an analogous position in any polypeptide based on a sequence alignment (such as prepared by BLAST or other approach disclosed herein or known in the art) to GR α , which are not forth herein for convenience.

[0319] As used in the following discussion, the terms "engineered NR", "engineered NR LDB", "NR mutant", and "NR LBD mutant" refers to polypeptides having amino acid sequences that contain at least one mutation in the wild-type sequence, including at an analogous position in any polypeptide based on a sequence alignment to GR α . The terms also refer to NR and NR LBD polypeptides which are capable of exerting a biological effect in that they comprise all or a part of the amino acid sequence of an engineered mutant polypeptide of the present invention, or cross-react with antibodies raised against an engineered mutant polypeptide, or retain all or some or an enhanced degree of the biological activity of the engineered mutant amino acid sequence or protein. Such biological activity can include the binding of small molecules in general, the binding of glucocorticoids in particular and even more particularly the binding of dexamethasone.

[0320] The terms "engineered NR LBD" and "NR LBD mutant" also includes analogs of an engineered NR polypeptide or NR LBD mutant polypeptide. By "analog" is intended that a DNA or polypeptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some or an enhanced degree of the biological activity of those sequences. Analogs can be derived from genomic nucleotide sequences or from other organisms, or can be created synthetically. Those of skill in the art will appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct mutant analogs. There is no need for an engineered mutant polypeptide to comprise all or substantially all of the amino acid sequence of the wild type polypeptide (e.g. SEQ ID NOs: 2, 4, 6 and 8). Shorter or longer sequences are anticipated to be of use in the invention; shorter sequences are herein referred to as "segments". Thus, the terms "engineered NR LBD" and "NR LBD mutant" also includes fusion, chimeric or recombinant engineered NR LBD or NR LBD mutant polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein above.

X.D. Sequence Similarity and Identity

[0321] As used herein, the term "substantially similar" as applied to GR means that a particular sequence varies from nucleic acid sequence of any of SEQ ID NOs: 1, 3, 5, or 7, or the amino acid sequence of any of SEQ ID NOs: 2, 4, 6 or 8 by one or more deletions, substitutions, or additions, the net effect of which is to retain at least some of biological activity of the natural gene, gene product, or sequence. Such sequences include "mutant" or "polymorphic" sequences, or sequences in which the biological activity and/or the physical properties are altered to some degree but retains at least some or an enhanced degree of the original biological activity and/or physical properties. In determining nucleic acid sequences, all subject nucleic acid sequences capable of encoding substantially similar amino acid sequences are considered to be substantially similar to a reference nucleic acid sequence, regardless of differences in codon sequences or substitution of equivalent amino acids to create biologically functional equivalents.

X.D.1. Sequences That are Substantially Identical to an Engineered NR or NR LBD Mutant Sequence of the Present Invention

[0322] Nucleic acids that are substantially identical to a nucleic acid sequence of an engineered NR or NR LBD mutant of the present invention, e.g. allelic variants, genetically altered versions of the gene, etc., bind to an engineered NR or NR LBD mutant sequence under stringent hybridization conditions. By using probes, particularly labeled probes of DNA sequences, one can isolate homologous or related genes. The source of homologous genes can be any species, e.g. primate species; rodents, such as rats and mice, canines, felines, bovines, equines, yeast, nematodes, etc.

[0323] Between mammalian species, e.g. human and mouse, homologs have substantial sequence similarity, i.e. at least 75% sequence identity between nucleotide sequences. Sequence similarity is calculated based on a reference sequence, which can be a subset of a larger sequence, such as a conserved motif, coding region, flanking region, etc. A reference sequence will usually be at least about 18 nt long, more usually at least about 30 nt long, and can extend to the complete sequence that is being compared. Algorithms for sequence analysis are known in the art, such as BLAST, described in Altschul et al., (1990) *J. Mol. Biol.* 215:403-10. Software for performing BLAST analyses is publicly available through the National Center for Biotechnology Information (<http://www.ncbi.nlm.nih.gov/>).

[0324] This algorithm involves first identifying high scoring sequence pairs (HSPs) by identifying short words of length W in the query sequence, which either match or satisfy some positive-valued threshold score T when aligned with a word of the same length in a database sequence. T is referred to as the neighborhood word score threshold. These initial neighborhood word hits act as seeds for initiating searches to find longer HSPs containing them. The word hits are then extended in both directions along each sequence for as far as the cumulative alignment score can be increased. Cumulative scores are calculated using, for nucleotide sequences, the parameters M (reward score for a pair of matching residues; always > 0) and N (penalty score for mismatching residues; always < 0). For amino acid sequences, a scoring matrix is used to calculate the cumulative score. Extension of the word hits in each direction are halted when the cumulative alignment score falls off by the quantity X from its maximum achieved value, the cumulative score goes to zero or below due to the accumulation of one or more negative-scoring residue alignments, or the end of either sequence is reached. The BLAST algorithm parameters W, T, and X determine the sensitivity and speed of the alignment. The BLASTN program (for nucleotide sequences) uses as defaults a wordlength W=11, an expectation E=10, a cutoff of 100, M=5, N=-4, and a comparison of both strands. For amino acid sequences, the BLASTP program uses as defaults a wordlength (W) of 3, an expectation (E) of 10, and the BLOSUM62 scoring matrix. See Henikoff & Henikoff, (1989) *Proc. Natl. Acad. Sci. U.S.A.* 89:10915.

[0325] In addition to calculating percent sequence identity, the BLAST algorithm also performs a statistical analysis of the similarity between two sequences. See, e.g., Karlin & Altschul, (1993) *Proc. Natl. Acad. Sci. U.S.A.* 90:5873-5887. One measure of similarity provided by the BLAST algorithm is the smallest sum probability (P(N)), which provides an indication of the probability by which a match between two nucleotide or amino acid sequences would occur by chance. For example, a test nucleic acid sequence is considered similar to a reference sequence if the smallest sum probability in a comparison of the test nucleic acid sequence to the reference nucleic acid sequence is less than about 0.1, more preferably less than about 0.01, and most preferably less than about 0.001.

[0326] Percent identity or percent similarity of a DNA or peptide sequence can be determined, for example, by comparing sequence information using the GAP computer program, available from the University of Wisconsin Geneticist Computer Group. The GAP program utilizes the alignment method of Needleman et al., (1970) *J. Mol. Biol.* 48:443, as revised by Smith et al., (1981) *Adv. Appl. Math.* 2:482. Briefly, the GAP program defines similarity as the number of aligned symbols (i.e., nucleotides or amino acids) that are similar, divided by the total number of symbols in the shorter of the two sequences. The preferred parameters for the GAP program are the default parameters, which do not impose a penalty for end gaps. See, e.g., Schwartz et al. (eds.), (1979), Atlas of Protein Sequence and Structure, National Biomedical Research Foundation, pp. 357-358, and Gribskov et al., (1986) *Nucl. Acids. Res.* 14:6745.

[0327] The term "similarity" is contrasted with the term "identity". Similarity is defined as above; "identity", however, means a nucleic acid or amino acid sequence having the same amino acid at the same relative position in a given family member of a gene family. Homology and similarity are generally viewed as broader terms than the term identity. Biochemically similar amino acids, for example leucine/isoleucine or glutamate/aspartate, can be present at the same position--these are not identical per se, but are biochemically "similar." As disclosed herein, these are referred to as conservative differences or conservative substitutions. This differs from a conservative mutation at the DNA level, which changes the nucleotide sequence without making a change in the encoded amino acid, e.g. TCC to TCA, both of which encode serine.

[0328] As used herein, DNA analog sequences are "substantially identical" to specific DNA sequences disclosed herein if: (a) the DNA analog sequence is derived from coding regions of the nucleic acid sequence shown in any one of SEQ ID NOs: 1, 3, 5 or 7 or (b) the DNA analog sequence is capable of hybridization with DNA sequences of (a) under stringent conditions and which encode a biologically active GR α or GR α LBD gene product; or (c) the DNA sequences are degenerate as a result of alternative genetic code to the DNA analog sequences defined in (a) and/or

(b). Substantially identical analog proteins and nucleic acids will have between about 70% and 80%, preferably between about 81% to about 90% or even more preferably between about 91% and 99% sequence identity with the corresponding sequence of the native protein or nucleic acid. Sequences having lesser degrees of identity but comparable biological activity are considered to be equivalents.

5 [0329] As used herein, "stringent conditions" means conditions of high stringency, for example 6X SSC, 0.2% polyvinylpyrrolidone, 0.2% Ficoll, 0.2% bovine serum albumin, 0.1% sodium dodecyl sulfate, 100 µg/ml salmon sperm DNA and 15% formamide at 68°C. For the purposes of specifying additional conditions of high stringency, preferred conditions are salt concentration of about 200 mM and temperature of about 45°C. One example of such stringent conditions is hybridization at 4X SSC, at 65°C, followed by a washing in 0.1XSSC at 65°C for one hour. Another exemplary

10 stringent hybridization scheme uses 50% formamide, 4X SSC at 42°C.

[0330] In contrast, nucleic acids having sequence similarity are detected by hybridization under lower stringency conditions. Thus, sequence identity can be determined by hybridization under lower stringency conditions, for example, at 50°C or higher and 0.1X SSC (9 mM NaCl/0.9 mM sodium citrate) and the sequences will remain bound when subjected to washing at 55°C in 1X SSC.

15 [0331] As used herein, the term "complementary sequences" means nucleic acid sequences that are base-paired according to the standard Watson-Crick complementarity rules. The present invention also encompasses the use of nucleotide segments that are complementary to the sequences of the present invention.

[0332] Hybridization can also be used for assessing complementary sequences and/or isolating complementary nucleotide sequences. As discussed above, nucleic acid hybridization will be affected by such conditions as salt concentration, temperature, or organic solvents, in addition to the base composition, length of the complementary strands, and the number of nucleotide base mismatches between the hybridizing nucleic acids, as will be readily appreciated by those skilled in the art. Stringent temperature conditions will generally include temperatures in excess of about 30°C, typically in excess of about 37°C, and preferably in excess of about 45°C. Stringent salt conditions will ordinarily be less than about 1,000 mM, typically less than about 500 mM, and preferably less than about 200 mM. However, the combination of parameters is much more important than the measure of any single parameter. See, e.g., Wetmur & Davidson, (1968) *J. Mol. Biol.* 31:349-70. Determining appropriate hybridization conditions to identify and/or isolate sequences containing high levels of homology is well known in the art. See, e.g., Sambrook et al., (1989) *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor, New York.

30 X.D.2. Functional Equivalents of an Engineered NR, SR or GR or NR, SR, GR LBD Mutant Nucleic Acid Sequence of the Present Invention

[0333] As used herein, the term "functionally equivalent codon" is used to refer to codons that encode the same amino acid, such as the ACG and AGU codons for serine. For example, GRα or GRα LBD-encoding nucleic acid sequences comprising any one of SEQ ID NOs: 1, 3, 5 or 7 that have functionally equivalent codons are covered by the present invention. Thus, when referring to the sequence example presented in SEQ ID NOs: 1, 3, 5 or 7, applicants provide substitution of functionally equivalent codons into the sequence example of in SEQ ID NOs: 1, 3, 5 or 7. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

40 [0334] It will also be understood by those of skill in the art that amino acid and nucleic acid sequences can include additional residues, such as additional N-terminal amino acids or 5' or 3' nucleic acid sequences, and yet still be essentially as set forth in one of the sequences disclosed herein, so long as the sequence retains biological protein activity where polypeptide expression is concerned. The addition of terminal sequences particularly applies to nucleic acid sequences which can, for example, include various non-coding sequences flanking either of the 5' or 3' portions of the coding region or can include various internal sequences, i.e., introns, which are known to occur within genes.

45 X.D.3. Biological Equivalents

[0335] The present invention envisions and includes biological equivalents of an engineered NR or NR LBD mutant polypeptide of the present invention. The term "biological equivalent" refers to proteins having amino acid sequences which are substantially identical to the amino acid sequence of an engineered NR LBD mutant of the present invention and which are capable of exerting a biological effect in that they are capable of binding small molecules or cross-reacting with anti-NR or NR LBD mutant antibodies raised against an engineered mutant NR or NR LBD polypeptide of the present invention.

55 [0336] For example, certain amino acids can be substituted for other amino acids in a protein structure without appreciable loss of interactive capacity with, for example, structures in the nucleus of a cell. Since it is the interactive capacity and nature of a protein that defines that protein's biological functional activity, certain amino acid sequence substitutions can be made in a protein sequence (or the nucleic acid sequence encoding it) to obtain a protein with the

same, enhanced, or antagonistic properties. Such properties can be achieved by interaction with the normal targets of the protein, but this need not be the case, and the biological activity of the invention is not limited to a particular mechanism of action. It is thus in accordance with the present invention that various changes can be made in the amino acid sequence of an engineered NR or NR LBD mutant polypeptide of the present invention or its underlying nucleic acid sequence without appreciable loss of biological utility or activity.

[0337] Biologically equivalent polypeptides, as used herein, are polypeptides in which certain, but not most or all, of the amino acids can be substituted. Thus, when referring to the sequence examples presented in any of SEQ ID NOs: 1, 3, 5 and 7, applicants envision substitution of codons that encode biologically equivalent amino acids, as described herein, into a sequence example of SEQ ID NOs: 1, 3, 5 and 7, respectively. Thus, applicants are in possession of amino acid and nucleic acid sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

[0338] Alternatively, functionally equivalent proteins or peptides can be created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, based on considerations of the properties of the amino acids being exchanged, e.g. substitution of Ile for Leu. Changes designed by man can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the antigenicity of the protein or to test an engineered mutant polypeptide of the present invention in order to modulate lipid-binding or other activity, at the molecular level.

[0339] Amino acid substitutions, such as those which might be employed in modifying an engineered mutant polypeptide of the present invention are generally, but not necessarily, based on the relative similarity of the amino acid side-chain substituents, for example, their hydrophobicity, hydrophilicity, charge, size, and the like. An analysis of the size, shape and type of the amino acid side-chain substituents reveals that arginine, lysine and histidine are all positively charged residues; that alanine, glycine and serine are all of similar size; and that phenylalanine, tryptophan and tyrosine all have a generally similar shape. Therefore, based upon these considerations, arginine, lysine and histidine; alanine, glycine and serine; and phenylalanine, tryptophan and tyrosine; are defined herein as biologically functional equivalents. Those of skill in the art will appreciate other biologically functionally equivalent changes. It is implicit in the above discussion, however, that one of skill in the art can appreciate that a radical, rather than a conservative substitution is warranted in a given situation. Non-conservative substitutions in engineered mutant LBD polypeptides of the present invention are also an aspect of the present invention.

[0340] In making biologically functional equivalent amino acid substitutions, the hydropathic index of amino acids can be considered. Each amino acid has been assigned a hydropathic index on the basis of their hydrophobicity and charge characteristics, these are: isoleucine (+ 4.5); valine (+ 4.2); leucine (+ 3.8); phenylalanine (+ 2.8); cysteine (+ 2.5); methionine (+ 1.9); alanine (+ 1.8); glycine (-0.4); threonine (-0.7); serine (-0.8); tryptophan (-0.9); tyrosine (-1.3); proline (-1.6); histidine (-3.2); glutamate (-3.5); glutamine (-3.5); aspartate (-3.5); asparagine (-3.5); lysine (-3.9); and arginine (-4.5).

[0341] The importance of the hydropathic amino acid index in conferring interactive biological function on a protein is generally understood in the art (Kyte & Doolittle, (1982), J. Mol. Biol. 157:105-132, incorporated herein by reference). It is known that certain amino acids can be substituted for other amino acids having a similar hydropathic index or score and still retain a similar biological activity. In making changes based upon the hydropathic index, the substitution of amino acids whose hydropathic indices are within ± 2 of the original value is preferred, those which are within ± 1 of the original value are particularly preferred, and those within ± 0.5 of the original value are even more particularly preferred.

[0342] It is also understood in the art that the substitution of like amino acids can be made effectively on the basis of hydrophilicity. U.S. Patent No. 4,554,101, incorporated herein by reference, states that the greatest local average hydrophilicity of a protein, as governed by the hydrophilicity of its adjacent amino acids, correlates with its immunogenicity and antigenicity, i.e. with a biological property of the protein. It is understood that an amino acid can be substituted for another having a similar hydrophilicity value and still obtain a biologically equivalent protein.

[0343] As detailed in U.S. Patent No. 4,554,101, the following hydrophilicity values have been assigned to amino acid residues: arginine (+3.0); lysine (+ 3.0); aspartate (+ 3.0 \pm 1); glutamate (+ 3.0 \pm 1); serine (+ 0.3); asparagine (+ 0.2); glutamine (+ 0.2); glycine (0); threonine (-0.4); proline (-0.5 \pm 1); alanine (-0.5); histidine (-0.5); cysteine (-1.0); methionine (-1.3); valine (-1.5); leucine (-1.8); isoleucine (-1.8); tyrosine (-2.3); phenylalanine (-2.5); tryptophan (-3.4).

[0344] In making changes based upon similar hydrophilicity values, the substitution of amino acids whose hydrophilicity values are within ± 2 of the original value is preferred, those which are within ± 1 of the original value are particularly preferred, and those within ± 0.5 of the original value are even more particularly preferred.

[0345] While discussion has focused on functionally equivalent polypeptides arising from amino acid changes, it will be appreciated that these changes can be effected by alteration of the encoding DNA, taking into consideration also that the genetic code is degenerate and that two or more codons can code for the same amino acid.

[0346] Thus, it will also be understood that this invention is not limited to the particular amino acid and nucleic acid sequences of any of SEQ ID NOs: 1-11. Recombinant vectors and isolated DNA segments can therefore variously

include an engineered NR or NR LBD mutant polypeptide-encoding region itself, include coding regions bearing selected alterations or modifications in the basic coding region, or include larger polypeptides which nevertheless comprise an NR or NR LBD mutant polypeptide-encoding regions or can encode biologically functional equivalent proteins or polypeptides which have variant amino acid sequences. Biological activity of an engineered NR or NR LBD mutant

5 polypeptide can be determined, for example, by transcription assays known to those of skill in the art.
[0347] The nucleic acid segments of the present invention, regardless of the length of the coding sequence itself, can be combined with other DNA sequences, such as promoters, enhancers, polyadenylation signals, additional restriction enzyme sites, multiple cloning sites, other coding segments, and the like, such that their overall length can vary considerably. It is therefore contemplated that a nucleic acid fragment of almost any length can be employed, with
 10 the total length preferably being limited by the ease of preparation and use in the intended recombinant DNA protocol. For example, nucleic acid fragments can be prepared which include a short stretch complementary to a nucleic acid sequence set forth in any of SEQ ID NOs: 1, 3, 5 and 7, such as about 10 nucleotides, and which are up to 10,000 or 5,000 base pairs in length. DNA segments with total lengths of about 4,000, 3,000, 2,000, 1,000, 500, 200, 100, and about 50 base pairs in length are also useful.

15 **[0348]** The DNA segments of the present invention encompass biologically functional equivalents of engineered NR, or NR LBD mutant polypeptides. Such sequences can arise as a consequence of codon redundancy and functional equivalency that are known to occur naturally within nucleic acid sequences and the proteins thus encoded. Alternatively, functionally equivalent proteins or polypeptides can be created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, based on considerations of the properties of the
 20 amino acids being exchanged. Changes can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the antigenicity of the protein or to test variants of an engineered mutant of the present invention in order to examine the degree of binding activity, or other activity at the molecular level. Various site-directed mutagenesis techniques are known to those of skill in the art and can be employed in the present invention.

25 **[0349]** The invention further encompasses fusion proteins and peptides wherein an engineered mutant coding region of the present invention is aligned within the same expression unit with other proteins or peptides having desired functions, such as for purification or immunodetection purposes.

[0350] Recombinant vectors form important further aspects of the present invention. Particularly useful vectors are those in which the coding portion of the DNA segment is positioned under the control of a promoter. The promoter can be that naturally associated with an NR gene, as can be obtained by isolating the 5' non-coding sequences located
 30 upstream of the coding segment or exon, for example, using recombinant cloning and/or PCR technology and/or other methods known in the art, in conjunction with the compositions disclosed herein.

[0351] In other embodiments, certain advantages will be gained by positioning the coding DNA segment under the control of a recombinant, or heterologous, promoter. As used herein, a recombinant or heterologous promoter is a promoter that is not normally associated with an NR gene in its natural environment. Such promoters can include
 35 promoters isolated from bacterial, viral, eukaryotic, or mammalian cells. Naturally, it will be important to employ a promoter that effectively directs the expression of the DNA segment in the cell type chosen for expression. The use of promoter and cell type combinations for protein expression is generally known to those of skill in the art of molecular biology (see, e.g., Sambrook et al., (1989) Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Laboratory, New York, United States of America, specifically incorporated herein by reference). The promoters employed can be
 40 constitutive or inducible and can be used under the appropriate conditions to direct high level expression of the introduced DNA segment, such as is advantageous in the large-scale production of recombinant proteins or peptides. One preferred promoter system contemplated for use in high-level expression is a T7 promoter-based system.

X.E. Antibodies to an Engineered NR or NR LBD Mutant Polypeptide of the Present Invention

45 **[0352]** The present invention also provides an antibody that specifically binds a engineered NR or NR LBD mutant polypeptide and methods to generate same. The term "antibody" indicates an immunoglobulin protein, or functional portion thereof, including a polyclonal antibody, a monoclonal antibody, a chimeric antibody, a single chain antibody, Fab fragments, and a Fab expression library. "Functional portion" refers to the part of the protein that binds a molecule
 50 of interest. In a preferred embodiment, an antibody of the invention is a monoclonal antibody. Techniques for preparing and characterizing antibodies are well known in the art (see, e.g., Harlow & Lane, (1988) Antibodies: A Laboratory Manual, Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York, United States of America). A monoclonal antibody of the present invention can be readily prepared through use of well-known techniques such as the hybridoma techniques exemplified in U.S. Patent No 4,196,265 and the phage-displayed techniques disclosed in U.S. Patent No.
 55 5,260,203.

[0353] The phrase "specifically (or selectively) binds to an antibody", or "specifically (or selectively) immunoreactive with", when referring to a protein or peptide, refers to a binding reaction which is determinative of the presence of the protein in a heterogeneous population of proteins and other biological materials. Thus, under designated immunoassay

conditions, the specified antibodies bind to a particular protein and do not show significant binding to other proteins present in the sample. Specific binding to an antibody under such conditions can require an antibody that is selected for its specificity for a particular protein. For example, antibodies raised to a protein with an amino acid sequence encoded by any of the nucleic acid sequences of the invention can be selected to obtain antibodies specifically immunoreactive with that protein and not with unrelated proteins.

[0354] The use of a molecular cloning approach to generate antibodies, particularly monoclonal antibodies, and more particularly single chain monoclonal antibodies, are also provided. The production of single chain antibodies has been described in the art. See, e.g., U.S. Patent No. 5,260,203. For this approach, combinatorial immunoglobulin phagemid libraries are prepared from RNA isolated from the spleen of the immunized animal, and phagemids expressing appropriate antibodies are selected by panning on endothelial tissue. The advantages of this approach over conventional hybridoma techniques are that approximately 10^4 times as many antibodies can be produced and screened in a single round, and that new specificities are generated by heavy (H) and light (L) chain combinations in a single chain, which further increases the chance of finding appropriate antibodies. Thus, an antibody of the present invention, or a "derivative" of an antibody of the present invention, pertains to a single polypeptide chain binding molecule which has binding specificity and affinity substantially similar to the binding specificity and affinity of the light and heavy chain aggregate variable region of an antibody described herein.

[0355] The term "immunochemical reaction", as used herein, refers to any of a variety of immunoassay formats used to detect antibodies specifically bound to a particular protein, including but not limited to competitive and non-competitive assay systems using techniques such as radioimmunoassays, ELISA (enzyme linked immunosorbent assay), "sandwich" immunoassays, immunoradiometric assays, gel diffusion precipitation reactions, immunodiffusion assays, *in situ* immunoassays (e.g., using colloidal gold, enzyme or radioisotope labels), western blots, precipitation reactions, agglutination assays (e.g., gel agglutination assays, hemagglutination assays), complement fixation assays, immunofluorescence assays, protein A assays, and immunoelectrophoresis assays, etc. See Harlow & Lane, (1988) Antibodies: A Laboratory Manual, Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York, United States of America, for a description of immunoassay formats and conditions.

X.F. Method for Detecting an Engineered NR or NR LBD Mutant Polypeptide or an Nucleic Acid Molecule Encoding the Same

[0356] In another aspect of the invention, a method is provided for detecting a level of an engineered NR or NR LBD mutant polypeptide using an antibody that specifically recognizes an engineered NR or NR LBD mutant polypeptide, or portion thereof. In a preferred embodiment, biological samples from an experimental subject and a control subject are obtained, and an engineered NR or NR LBD mutant polypeptide is detected in each sample by immunochemical reaction with the antibody. More preferably, the antibody recognizes amino acids of any one of SEQ ID NOs: 2, 4, 6 and 8, and is prepared according to a method of the present invention for producing such an antibody.

[0357] In one embodiment, an antibody is used to screen a biological sample for the presence of an engineered NR or NR LBD mutant polypeptide. A biological sample to be screened can be a biological fluid such as extracellular or intracellular fluid, or a cell or tissue extract or homogenate. A biological sample can also be an isolated cell (e.g., in culture) or a collection of cells such as in a tissue sample or histology sample. A tissue sample can be suspended in a liquid medium or fixed onto a solid support such as a microscope slide. In accordance with a screening assay method, a biological sample is exposed to an antibody immunoreactive with an engineered NR or NR LBD mutant polypeptide whose presence is being assayed, and the formation of antibody-polypeptide complexes is detected. Techniques for detecting such antibody-antigen conjugates or complexes are well known in the art and include but are not limited to centrifugation, affinity chromatography and the like, and binding of a labeled secondary antibody to the antibody-candidate receptor complex.

[0358] In another aspect of the invention, a method is provided for detecting a nucleic acid molecule that encodes an engineered NR or NR LBD mutant polypeptide. According to the method, a biological sample having nucleic acid material is procured and hybridized under stringent hybridization conditions to an engineered NR or NR LBD mutant polypeptide-encoding nucleic acid molecule of the present invention. Such hybridization enables a nucleic acid molecule of the biological sample and an engineered NR or NR LBD mutant polypeptide encoding-nucleic acid molecule to form a detectable duplex structure. Preferably, the an engineered NR or NR LBD mutant polypeptide encoding-nucleic acid molecule includes some or all nucleotides of any one of SEQ ID NOs: 1, 3, 5 and 7. It is also preferable that the biological sample comprises human nucleic acid material.

XI. The Role of the Three-Dimensional Structure of the GR α LBD in Solving Additional NR, SR or GR Crystals

[0359] Because polypeptides can crystallize in more than one crystal form, the structural coordinates of a GR α LBD, or portions thereof, as provided by the present invention, are particularly useful in solving the structure of other crystal

forms of GR α and the crystalline forms of other NRs, SRs and GRs. The coordinates provided in the present invention can also be used to solve the structure of NR and NR LBD mutants (such as those described in Sections IX and X above), NR LBD co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of a NR.

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XI.A. Determining the Three-Dimensional Structure of a Polypeptide Using the Three-Dimensional Structure of the GR α LBD as a Template in Molecular Replacement

[0360] One method that can be employed for the purpose of solving additional GR crystal structures is molecular replacement. See generally, Rossmann (ed.), (1972) The Molecular Replacement Method, Gordon & Breach, New York, New York, United States of America. In the molecular replacement method, the unknown crystal structure, whether it is another crystal form of a GR α or a GR α LBD, (i.e. a GR α or a GR α LBD mutant), or an NR or an NR LBD polypeptide complexed with another compound (a "co-complex"), or the crystal of some other protein with significant amino acid sequence homology to any functional region of the GR α LBD, can be determined using the GR α LBD structure coordinates provided in Table 2. This method provides an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

[0361] In addition, in accordance with this invention, NR and NR LBD mutants can be crystallized in complex with known modulators. The crystal structures of a series of such complexes can then be solved by molecular replacement and compared with that of the wild-type NR or the wild-type NR LBD. Potential sites for modification within the various binding sites of the enzyme can thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between the GR α LBD and a chemical entity or compound.

[0362] All of the complexes referred to in the present disclosure can be studied using X-ray diffraction techniques (See, e.g., Blundell & Johnson (1985) *Method. Enzymol.*, 114A & 115B, (Wyckoff et al., eds.), Academic Press; McRee, (1993) Practical Protein Crystallography, Academic Press, New York, New York) and can be refined using computer software, such as the X-PLOR™ program (Brünger, (1992) *X-PLOR, Version 3.1. A System for X-ray Crystallography and NMR*, Yale University Press, New Haven, Connecticut; X-PLOR is available from Accelrys of San Diego, California, United States of America) and the XTAL-VIEW program (McRee, (1992) *J. Mol. Graphics* 10:44-46; McRee, (1993) Practical Protein Crystallography, Academic Press, San Diego, California, United States of America). This information can thus be used to optimize known classes of GR and GR LBD modulators, and more importantly, to design and synthesize novel classes of GR and GR LBD modulators.

Laboratory Examples

[0363] The following Laboratory Examples have been included to illustrate preferred modes of the invention. Certain aspects of the following Laboratory Examples are described in terms of techniques and procedures found or contemplated by the present inventors to work well in the practice of the invention. These Laboratory Examples are exemplified through the use of standard laboratory practices of the inventors. In light of the present disclosure and the general level of skill in the art, those of skill will appreciate that the following Laboratory Examples are intended to be exemplary only and that numerous changes, modifications and alterations can be employed without departing from the spirit and scope of the invention.

Laboratory Example 1

Expression Of a GR α Polypeptide

[0364] BL21(DE3) cells (Novagen/Invitrogen, Inc., Carlsbad, California, United States of America) were transformed with the expression plasmid 6xHisGST-GR(521-777) F602S pET24 following established protocols. Following overnight incubation at 37°C a single colony was used to inoculate a 10 ml LB culture containing 50 µg/ml kanamycin (Sigma, St. Louis, Missouri, United States of America). The culture was grown for ~8 hrs at 30°C and then a 500µl aliquot was used to inoculate flasks containing 1 liter CIRCLE GROW™ media (Bio 101, Inc., Vista, California, United States of America) and the required antibiotic. The cells were then grown at 22°C to an OD600 between 2 and 3 and then cooled to 18°C. Following a 30 min equilibration at that temperature, dexamethasone (Spectrum Chemical Co., Gardena, California, United States of America) (50 or 100 µM final concentration) was added. Induction of expression was achieved by adding IPTG (BACHEM, Philadelphia, Pennsylvania, United States of America) (final concentration 1 mM) to the cultures. Expression at 18°C was continued for ~20 hrs. Cells were then harvested and frozen at -80°C.

[0365] In another example, GR LBD was expressed in the presence of 50 or 100 µM FP. This approach eliminated the step of exchanging dexamethasone with fluticasone propionate during the purification process. The GR LBD/FP

complex that was formed by expressing the GR LBD in the presence of 50 or 100 μ M FP also formed crystals.

Laboratory Example 2

5 Purification Of a GR LBD (521-777) F602S Polypeptide Bound to Fluticasone Propionate

[0366] Approximately 37 g of cells were resuspended in 500 mL lysis buffer (50mM Tris pH =8.0, 150 mM NaCl, 2M urea, and 30 μ M fluticasone propionate) and lysed by passing 3 times through a Rannie APV Lab 2000 homogenizer (Rannie APV, Copenhagen, Denmark). The lysate was subjected to centrifugation (30 minutes, 20,000g, 4°C). The
10 cleared supernatant was filtered through coarse pre-filters and 50 mM Tris, pH= 8.0, containing 150 mM NaCl and 1M imidazole was added to obtain a final imidazole concentration of 50mM. This lysate was loaded onto a XK-26 column (Pharmacia, Peapack, New Jersey) packed with Sepharose [Ni²⁺ charged] chelation resin (Pharmacia, Peapack, New Jersey) and pre-equilibrated with lysis buffer supplemented with 50mM imidazole. Following loading, the column was washed to baseline absorbance with equilibration buffer. This was followed by a linear (0 to 10%) glycerol and (2M to
15 0M) urea gradient. For elution the column was developed with a linear gradient from 50 to 500 mM imidazole in 50mM Tris pH =8.0, 150 mM NaCl, 10% glycerol and 30 μ M fluticasone propionate. Column fractions of interest were pooled and 500 units of thrombin protease (Amersham Pharmacia Biotech, Piscataway, New Jersey, United States of America) were added for the cleavage of the fusion protein. This solution was then dialyzed against 1 liter of 50 mM Tris pH = 8.0, 150 mM NaCl, 10% glycerol and 30 μ M fluticasone propionate for ~24 hrs at 4°C. The digested protein sample
20 was filtered and then reloaded onto a fresh (previously equilibrated) Ni⁺⁺ charged column. The cleaved GR LBD was collected in the flow-through fraction. The diluted protein sample was concentrated with CENTRIPREP™ 10K centrifugal filtration devices (Amicon/Millipore, Bedford, Massachusetts, United States of America) to a volume of 45ml and then diluted 5 fold with 50 mM Tris pH=8.0, 10 % glycerol, 10 mM DTT, 0.5 mM EDTA and 30 μ M fluticasone propionate. The sample was then loaded onto a pre-equilibrated XK-26 column (Pharmacia, Peapack, New Jersey, United States
25 of America) packed with Poros HQ resin (PerSeptive Biosystems, Framingham, Massachusetts, United States of America). The cleaved GR LBD was collected in the flowthrough. The NaCl concentration was adjusted to 500mM and the purified protein was concentrated to ~15 mg/ml using the CENTRIPREP™ 10K centrifugal filtration devices and then frozen at -80°C.

[0367] Figure 1 is an autoradiogram of a polyacrylamide gel summarizing the isolation of a GR mutant of the present invention. In this figure, Lane 1 contains the insoluble pellet fraction. Lane 2 contains the soluble supernatant fraction. Lane 3 contains pooled eluent from the initial Ni²⁺ column. Lane 4 contains the sample after thrombin digestion. Lane 5 contains the flow through fraction after reload of the Ni²⁺ column. Lane 6 contains the protein after anion exchange. The positions of molecular mass (kDa) markers are indicated on the left side of the figure.

35 Laboratory Example 3

Preparation of a GR/TIF2/Fluticasone Propionate (FP) Complex

[0368] The GR/TIF2/FP complex was prepared by adding a 1.2-fold excess of a TIF2 peptide containing sequence of KENALLRYLLDKDD (SEQ ID NO: 9) during the buffer exchange step as described below. The above complex was
40 concentrated then diluted 1:1 with a buffer containing 500 mM NH₄OAc, 50 mM Tris, pH 8.0, 10% glycerol, 10 mM dithiothreitol (DTT), 0.5mM EDTA and 0.05% β -octyl-glucoside and concentrated to 1 ml. The complex was diluted 1: 9 with the above buffer and slowly concentrated to 7.5 mg/ml in the presence of an additional 1.2 fold excess of a TIF2 peptide (residues 740-753), aliquoted and stored at -80 °C.

45 Laboratory Example 4

Crystallization and Data Collection

[0369] The GR/TIF2/FP crystals were grown at room temperature in hanging drops containing 3.0 μ l of the above protein-ligand solutions, and 0.5 μ l of well buffer (60mM Bis-Tris-Propane, PH 7.5-8.5, and 1.5-1.7 M magnesium sulfate). Crystals appeared overnight and continuously grew to a size of up to 300 microns within several weeks. Before data collection, crystals were flash frozen in liquid nitrogen.

[0370] The GR/TIF2/FP crystals formed in the P6₁ space group, with a = b = 127.656 Å, c = 87.725 Å, $\alpha = \beta = 90^\circ$,
55 and $\gamma = 120^\circ$. Each asymmetry unit contains two molecules of the GR LBD with 58% of solvent content. Data were collected using a MAR165 CCD detector at the 17BM of the Advanced Photon Source (APS) of Argonne National Laboratory in Chicago, Illinois, United States of America. The observed reflections were reduced, merged and scaled with DENZO and SCALEPACK in the HKL2000 package (Otwinowski et al., (1993) in Proceedings of the CCP4 Study

Weekend: Data Collection and Processing. (Sawyer et al., eds), pp. 56-62, SERC Daresbury Laboratory, England).

Laboratory Example 5

5 Structure Determination and Refinement

[0371] A model of GR/TIF2/FP complex was built based on the crystal structure of a GR/TIF2/dexamethasone complex ("the Dex structure"; coordinates of the Dex structure are presented in Table 3). This model was used in molecular replacement search with the CCP4 AmoRe program (Collaborative Computational Project Number 4, 1994; Navaza, 10 (1994) *Acta. Cryst.* A50:157-163) to determine the initial structure solutions. The calculated phase from the molecular replacement solutions was improved with solvent flattening, histogram matching and the two-fold noncrystallographic averaging as implemented in the CCP4 dm program, and produced a clear map for the GR LBD, the TIF2 peptide and the dexamethasone. Model building proceeded by employing the QUANTA software (Accelrys Inc., San Diego, California, United States of America), and refinement continued by employing the CNX software (Accelrys Inc., San Diego, 15 California, United States of America; Brunger et al., (1998) *Acta. Crystallogr.* D54:905-921) and multiple cycle of manual rebuilding. The statistics of the structure are summarized in Table 1.

Laboratory Example 6

20 Construction of a Docking Model for the Compound Benzoxazin-1-one Using a GR/FP/TIF2 Structure

[0372] The second subunit of the GR structure was selected as the initial crystal structure in which to model the benzoxazin-1-one compound and loaded into the display area of INSIGHTII (Accelrys Inc., San Diego, California, United States of America). As a reference, the crystal structure of the bound FP molecule in that subunit was loaded 25 into the same display area.

[0373] Initial coordinates of the benzoxazin-1-one were generated using CONCORD v4.0.4 (Tripos Inc., St. Louis, Missouri, United States of America). Conformers of the initial benzoxazin-1-one geometry were generated using the GROW algorithm available in MVP and optimized using CVFF as implemented in MVP (Lambert, (1997) in Practical Application of Computer-Aided Drug Design (Charifson, ed.), Marcel Dekker, New York, New York, United States of 30 America, pp. 243-303). Each of the resulting conformers were then hand-docked into the GR crystal structure and the best-fitting conformer was selected as the proposed binding conformation of the benzoxazin-1-one.

[0374] The initial GR/benzoxazin-1-one docking model complex was exported from the INSIGHTII software in the identical coordinate reference frame as the GR/FP crystal structure. Geometry optimization of the GR/benzoxazin-1-one complex was carried out using CVFF as implemented in MVP. All atoms in the complex remained fixed in space 35 except for those atoms contained in the benzoxazin-1-one and the initial GR structure that were within 6 angstroms of any atom in the benzoxazin-1-one. The CVFF energy terms were calculated using only those atoms within 16 angstroms of (and including) the benzoxazin-1-one. Geometry optimization of the protein-ligand complex was carried out using the conjugate gradient method as implemented in MVP and with a convergence criteria of a 0.1 change in the gradient.

[0375] Figure 9 depicts a docking model of a GR LBD with the benzoxazine-1-one ligand generated as described 40 hereinabove. Figure 10 depicts various interactions formed between the benzoxazin-1-one ligand and GR residues that comprising the binding pocket. Intermolecular distances are indicated in the figure. Figure 11 depicts the docking of the benzoxazin-1-one ligand with the GR binding pocket. The docking model comprises an expanded binding pocket, which, as Figure 11 shows, accommodates the *p*-fluorophenoilc side chain of the ligand.

[0376] Figure 12 a depiction of the overlay of the GR/Dex crystal structure (grey) with the GR/benzoxazin-1-one 45 model (white) comparing the geometries of the ligands and the relative locations of the amino acid side chains that compose the GR expanded binding pocket. Conformational differences between four residues (M560, M639, W642, and W735) allow for the additional volume of the expanded binding pocket. This added volume provides additional space in the binding pocket and allows the large *p*-fluorophenol group of the Schering compounds to extend beyond the dexamethasone D-ring and into this region. This added volume is observed in the GR/benzoxazin-1-one model 50 but is not observed in the GR/Dex structure.

[0377] Table 6 presents a subset of atomic coordinates of GR α in complex with benzoxazin-1-one obtained from modeling of the crystal structure of GR α in complex with FP.

Laboratory Example 7

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Construction of an AR Homology Model Bound with Bicalutamide Using a GR/FP/TIF2 Structure

[0378] A preferred method of constructing an NR homology model using a GR/TIF2/FP structure of the present

invention is disclosed. This method is illustrated by way of specific example, namely the construction of an AR homology model. Those of ordinary skill in the art will appreciate that although the method is presented in the context of generating an AR homology model, the method can be employed *mutatis mutandis* to generate homology models for all NRs.

[0379] In the formulation of an AR homology model based on the GR/TIF2/FP structure of the present invention, sequence alignments of the AR and GR LBDs were initially obtained using the alignment algorithm implemented in MVP (Lambert, (1997) in Practical Application of Computer-Aided Drug Design (Charifson, ed.), Marcel Dekker, New York, New York, United States of America, pp. 243-303). After three-dimensional alignment and coordinate translation of the GR/TIF2/FP crystal structure into a standard orientation using MVP, the second subunit of the GR/TIF2/FP structure was chosen for the AR homology model. Throughout the building the homology model, the Homology package in the INSIGHTII program (Accelrys Inc., San Diego, California, United States of America) was used to visualize the proteins, extract the LBD sequences, manually align the sequences, transform the amino acid residues, manually manipulate the amino acid sidechain conformers, and export the three-dimensional coordinates in appropriate file formats.

[0380] The second subunit of the GR/TIF2/FP structure was loaded into the display area of INSIGHTII along with the AR/DHT structure for comparison purposes. Using the Homology package, the GR/TIF2/FP and AR/DHT primary amino acid sequences were extracted from the crystal structures. The sequences were then manually aligned using Homology and by comparison with those alignments obtained using the MVP program.

[0381] The transformation of the amino acid residues was carried out and initial three-dimensional coordinates of the AR homology model were assigned using the AssignCoords method in the Homology modeling package. In assigning the coordinates of residues I672-K883 in the AR model, the corresponding coordinates of residues T531-D742 in the GR/TIF2/FP crystal structure were used. In assigning the coordinates of residues M886-H917 in the AR model, the corresponding coordinates of residues K744-H775 in the GR/TIF2/FP crystal structure were used. For the coordinates of residues S884-H885 in the AR model, the corresponding coordinates from the AR/DHT crystal structure were used. Manual modifications of amino acid side chain conformers were carried out after comparing the conformations of corresponding residues in the initial AR homology model and the AR/DHT crystal structure. The conformations of the following AR model residues were modified based on these comparisons: L880, M895, F697, K777, T877, and Q711.

[0382] Initial coordinates of bicalutamide were generated using CONCORD v4.0.4 (Tripos Inc., St. Louis, Missouri, United States of America). Conformers of the initial bicalutamide geometry were generated using the GROW algorithm available in MVP and optimized using CVFF as implemented in MVP. Each of the resulting conformers were then hand-docked into the initial AR homology model, and the best-fitting conformer was selected as the proposed binding conformation of bicalutamide.

[0383] The initial AR/bicalutamide homology model complex was exported from INSIGHTII in the identical coordinate reference frame as the GR/TIF2/FP crystal structure. Using MVP and the sequence alignments of GR and AR, the residue numbering of the initial AR model was corrected.

[0384] Geometry optimization of the AR/bicalutamide homology model complex was carried out using CVFF as implemented in MVP. All atoms in the complex remained fixed in space except for those atoms contained in bicalutamide and the initial AR model that were within 6 angstroms of any atom in bicalutamide. The CVFF energy terms were calculated using only those atoms within 16 angstroms of (and including) bicalutamide. Geometry optimization of the protein-ligand complex was carried out using the conjugate gradient method as implemented in MVP and with a convergence criteria of a 0.1 change in the gradient.

[0385] Figure 18A is a ribbon diagram that depicts an AR homology model formed using the GR/TIF2/FP structure of the present invention and the method disclosed hereinabove. The homology model comprises an expanded binding pocket similar to that observed in the GR/TIF2/FP structure of the present invention. The binding pocket is represented as a solid surface. By way of comparison, Figure 18B depicts a known AR/DHT LBD structure. This structure lacks an expanded binding pocket and cannot accommodate a bicalutamide ligand.

[0386] Figure 19 depicts a docking model of an AR LBD with the bicalutamide ligand generated as described hereinabove. The AF2, H3, H9 and H10 helices are labeled. Figure 20 depicts an orthogonal view of the structure depicted in Figure 19 and shows the orientation of the ligand in the binding pocket of AR. Figure 21, which is a stick diagram, depicts various interactions formed between the bicalutamide ligand and AR residues that comprising the binding pocket. Intermolecular distances are indicated in the figure. Figure 21 depicts the docking of the benzoxazin-1-one ligand with the AR binding pocket. Figure 22 is a ribbon diagram that shows the extension of the p-fluorophenyl group of the bicalutamide ligand into the expanded binding pocket formed in the AR-bicalutamide model.

[0387] Table 4 presents the atomic coordinates of AR in complex with bicalutamide obtained from homology modeling of the crystal structure coordinates of GR α in complex with FP.

Laboratory Example 8

Construction of a PR Homology Model Bound with RWJ-60130 Using a GR/TIF2/FP Crystal Structure

- 5 **[0388]** As noted, a GR/TIF2/FP structure of the present invention can be employed to construct a homology model of an NR. In the following section, a preferred method is presented by way of specific example, namely the construction of a PR homology model. In the following example, although PR is specifically recited, any NR can be employed and the following discussion is intended to illustrate one embodiment of this general method.
- 10 **[0389]** First, sequence alignments of the PR and GR LBDs were obtained using the alignment algorithm implemented in MVP. After three-dimensional alignment and coordinate translation of the GR/TIF2/FP crystal structure into a standard orientation using MVP, the second subunit of the GR/TIF2/FP structure was chosen for the PR homology modeling exercise.
- 15 **[0390]** The second subunit of the GR/TIF2/FP structure was loaded into the display area of INSIGHTII along with the PR/PG structure for comparison purposes. Using the Homology package, the GR/TIF2/FP and PR/PG primary amino acid sequences were extracted from the crystal structures. The sequences were then manually aligned using Homology and by comparison with those alignments obtained using the MVP program.
- 20 **[0391]** The transformation of the amino acid residues was carried out and initial three-dimensional coordinates of the PR homology model were assigned using the AssignCoords method in the Homology modeling package. In assigning the coordinates of residues Q682-Q897 and A900-K932 in the PR model, the corresponding coordinates of residues Q527-D742 and T744-Q776 in the GR/TIF2/FP crystal structure, respectively, were used. For the coordinates of residues S898-R899 in the PR model, the corresponding coordinates from the PR/PG crystal structure were used. Manual modifications of amino acid side chain conformers were carried out after comparing the conformations of corresponding residues in the initial PR homology model and the PR/PG crystal structure. The conformations of the following PR model residues were modified based on these comparisons: L799, W802, V823, N828, M909, L726, R740, S757, M759, and V760.
- 25 **[0392]** Initial coordinates of RWJ-60130 were generated using CONCORD v4.0.4. Conformers of the initial RWJ-60130 geometry were generated using the GROW algorithm available in MVP and optimized using CVFF as implemented in MVP. Each of the resulting conformers were then hand-docked into the initial PR homology model and the best-fitting conformer was selected as the proposed binding conformation of RWJ-60130.
- 30 **[0393]** The initial PR/RWJ-60130 homology model complex was exported from INSIGHTII in the identical coordinate reference frame as the GR/TIF2/FP crystal structure. Using MVP and the sequence alignments of GR and PR, the residue numbering of the initial PR model was corrected.
- 35 **[0394]** Geometry optimization of the PR/RWJ-60130 homology model complex was carried out using CVFF as implemented in MVP. All atoms in the complex remained fixed in space except for those atoms contained in RWJ-60130 and the initial PR model that were within 6 angstroms of any atom in RWJ-60130. The CVFF energy terms were calculated using only those atoms within 16 angstroms of (and including) RWJ-60130. Geometry optimization of the protein-ligand complex was carried out using the conjugate gradient method as implemented in MVP and with a convergence criteria of a 0.1 change in the gradient.
- 40 **[0395]** Figure 23A is a ribbon diagram depicting a PR LBD homology model formed using the method disclosed hereinabove and incorporating a GR/TIF2/FP structure of the present invention. The ligand binding pocket is depicted as a solid surface and comprises an expanded binding pocket, as seen in the GR/TIF2/FP structures of the present invention. On the other hand, Figure 23B depicts a known PR LBD structure, shown with the ligand progesterone positioned in the binding pocket. The PR/PG structure does not comprise an expanded binding pocket and cannot accommodate the ligand RWJ-60130.
- 45 **[0396]** Figure 24 is a ribbon diagram docking model depicting the association of the ligand RWJ-60130 with an AR LBD comprising an expanded binding pocket. The AR was modeled based on the GR/TIF2/FP structure of the present invention. Figure 25 is an orthogonal view of the structure depicted in Figure 24. Continuing, Figure 26 is a stick model of the interactions the RWJ-60130 ligand forms with the binding pocket of AR. Intermolecular distances are indicated. Figure 27 is an orthogonal view of the structure depicted in Figure 25. Figure 27 shows the extension of the p-fidodophenyl group of the RWJ-60130 ligand into the expanded binding pocket of the AR model. As noted, known AR models and structures that lack the expanded binding pocket cannot fully accommodate the RWJ-60130 ligand.
- 50 **[0397]** Table 5 presents atomic coordinates of PR in complex with RWJ-60130 obtained from homology modeling of the crystal structure coordinates of GR α in complex with FP.

Laboratory Example 9Construction of a Binding Model for A-222977 Using the GR/TIF2/FP Crystal Structure

- 5 [0398] The second subunit of the GR structure was selected as the initial crystal structure in which to model A-222977 and loaded into the display area of INSIGHTII. As a reference, the crystal structure of the bound FP molecule in that subunit was loaded into the same display area.
- [0399] Initial coordinates of A-222977 were generated using CONCORD v4.0.4. Conformers of the initial geometry were generated using the GROW algorithm available in MVP and optimized using CVFF as implemented in MVP. Each
10 of the resulting conformers were then hand-docked into the GR crystal structure and the best-fitting conformer was selected as the proposed binding conformation of A-222977.
- [0400] The initial GR/A-222977 model complex was exported from INSIGHTII in the identical coordinate reference frame as the GR/TIF2/FP crystal structure. Geometry optimization of the GR/A-222977 complex was carried out using CVFF as implemented in MVP. All atoms in the complex remained fixed in space except for those atoms contained in
15 A-222977 and the initial GR structure that were within 6 angstroms of any atom in A-222977. The CVFF energy terms were calculated using only those atoms within 16 angstroms of (and including) A-222977. Geometry optimization of the protein-ligand complex was carried out using the conjugate gradient method as implemented in MVP and with a convergence criteria of a 0.1 change in the gradient.
- [0401] Figure 13 is a docking model of the ligand A-222977 bound to GR. The GR is the GR/TIF2/FP structure that forms an aspect of the present invention. The model depicted in Figure 13 comprises the expanded binding pocket observed in the GR/TIF2/FP structure. Figure 15 is an orthogonal view of the structure of Figure 13. Figure 15 shows the extension of the methyl-sulfonyl-methoxyl-phenyl side chain of the A-222977 ligand into the expanded binding pocket formed in the GR structure. It is not possible to accurately dock the A-222977 ligand into the GR structure without the presence of the expanded binding pocket, due to the protrusion of the methyl-sulfonyl-methoxyl-phenyl
20 side chain beyond the bounds of the binding pocket. Figure 14 is a stick drawing that depicts the interaction between the residues of the ligand binding pocket of GR, which comprises the expanded binding pocket, and the A-222977 ligand.
- [0402] Figure 16 is an overlay of the GR/Dex structure with the GR/A-222977 structure. The ligands are represented as stick structures. Figure 16 illustrates several conformational differences between four residues (M560, M639, W642, and W735) contribute to the additional volume of the expanded binding pocket. The added volume encompassed by the expanded binding pocket provides additional space that allows the large methyl-sulfonyl-methoxyl-phenyl group of the A-222977 ligand to extend beyond the dexamethasone D-ring and into this region. Although this space is observed in the GR/A-222977 structure, it is not observed in the GR/Dex structure.
- [0403] Table 7 presents a subset of atomic coordinates of GR α in complex with A-222977 obtained from modeling
25 of the crystal structure of GR α in complex with FP.

Laboratory Example 11Construction of a Homology Model for MR Using a GR/TIF2/FP Structure

- 40 [0404] A model for the human MR LBD was built with the program MVP using the amino acid sequences of human MR (Genbank entry M16801.1), human GR (Genbank entry X03225.1), human PR (Genbank entry X51730.1) and human AR (SwissProt entry ANDR_HUMAN), together with the X-ray structures of GR bound to FP (Table 2) and PR bound to progesterone (Williams & Sigler, PDB entry 1A28). The MVP program was first used to align the amino acid sequences. This alignment, Figure 17, has a single gap, occurring in the GR sequence between GR Asp742 and Lys743, at a position corresponding to MR Ser949, PR Ser898 and AR Ser884. This gap lies in the loop between helix-10 and the AF2 helix. The alignment establishes a corresponding template residue in GR for each residue in the MR LBD except for MR Ser949, which lies in the single gap position. The A subunit of the GR/TIF2/FP complex, Table 2, as was selected as the primary template for the MR model. This structure provides coordinates for GR residues 523-777.
- 45 Using the residue correspondence from the sequence alignment, the MVP program generated coordinates for the backbone atoms of MR residues 729-948 and 950-984 by copying the corresponding coordinates in GR. The MVP program also copies coordinates for side-chain atoms in MR residues when the side-chain is identical to the corresponding residue in GR. Side-chains that differ from the corresponding side-chains in GR are built using standard bond lengths, angles and dihedral angles, but are built to adopt a conformation similar to that in GR when possible. Initially,
50 no coordinates were generated for Ser949. Energy calculations were used to refine the side-chain conformations. The FP ligand was included in the energy calculations to prevent protein side-chains from moving into the volume normally occupied by the ligand. The protein and ligand were protonated as expected at pH 7, and modeled with the CFF91 force field, as implemented in MVP. A grow calculation was used to generate alternative, low energy conformations for

the side-chains lying within 10Å of the FP ligand. No energy refinement was applied to side-chains lying more than 10Å from the FP ligand. The grow calculation used repeated cycles of torsional coordinate minimization on partially grown side-chain arrangements, followed by cartesian coordinate minimization to an RMS gradient of 0.3 kcal/Å². Backbone atoms, and side-chains that are identical in MR and GR, were held fixed during the energy calculations. After energy refinement of the side-chains in and around the ligand binding pocket, the helix-10/AF2 loop from PR was transplanted into the MR model. This transplant model was built by first superimposing the PR structure onto the GR and MR structures, replacing MR residues 945-950 with PR residues 894-904, renumbering these residues according to the MR numbering scheme, and mutating Ile947 to Arg, Gln948 to Glu, Arg950 to His and Ser953 to Lys. The entire model was then examined graphically within Insight-II. Side-chain conformations were adjusted graphically as necessary to avoid overlaps. Table 11 presents the three-dimensional coordinates for the MR homology model.

References

[0405] The references listed below as well as all references cited in the specification are incorporated herein by reference to the extent that they supplement, explain, provide a background for or teach methodology, techniques and/or compositions employed herein.

- Altschul *et al.*, (1990) *J. Mol. Biol.* 215: 403-10
 Apriletti *et al.*, (1995) *Protein Expres. Purif.* 6: 368-370
 Ausubel *et al.*, (1989) *Current Protocols in Molecular Biology*, Greene Publishing Associates and Wiley Interscience, New York
 Bartlett *et al.*, (1989) *Special Pub., Royal Chem. Soc.* 78: 182-96
 Beato, (1989) *Cell* 56:335-344
 Blundell & Johnson, (1985) *Method. Enzymol.* 114A & 115B, (Wyckoff *et al.*, eds.), Academic Press
 Bohlen, (1995) *J. Biol. Chem.* 270: 29433-29438
 Bohlen, (1998) *Mol. Cell. Biol.* 18: 3330-3339
 Bohm, (1992) *J. Comput. Aid. Mol. Des.* 6: 61-78
 Brooks *et al.*, (1983) *J. Comp. Chem.*, 8: 132
 Brünger, (1992) *X-PLOR, Version 3.1. A System for X-ray Crystallography and NMR*, Yale University Press, New Haven, Connecticut
 Caamano *et al.*, (1994) *Annal. NY Acad. Sci.* 746: 68-77
 Case *et al.*, (1997), AMBER 5, University of California, San Francisco, California, United States of America
 Cohen & Duke, (1984) *J. Immunol.* 152: 38-42
 Cohen *et al.*, (1990) *J. Meet. Chem.* 33: 883-94
 Creighton, (1983) *Proteins: Structures and Molecular Principles*, W.H. Freeman & Co., New York, United States of America
 Danielsen *et al.*, (1987) *Molec. Endocrinol.* 1: 816-822
 Danielsen *et al.*, (1989) *Cancer Res.* 49: 2286s-2291s
 DeBosscher *et al.*, (2000) *Proc. Natl. Acad. Sci. U. S. A.* 97: 3919-3924
 Drewes *et al.*, (1996) *Mol. Cell. Biol.* 16:925-31
 Ducruix & Geige, (1992) *Crystallization of Nucleic Acids and Proteins: A Practical Approach*, IRL Press, Oxford, England
 Dyda *et al.*, (1994) *Science* 266:1981-6
 Eastman-Reks & Vedeckis, (1986) *Cancer Res.* 46: 2457-2462
 Eisen *et al.*, (1994). *Proteins* 19:199-221
 Evans, (1989) in *Recent Progress in Hormone Research* (Clark, ed.) Vol. 45, pp. 1-27, Academic Press, San Diego, California, United States of America
 Evans, (1988) *Science* 240:889-895
 Freeman *et al.*, (2000) *Genes Dev.* 14: 422-434
 Gampe *et al.*, (2000) *Mol. Cell* 5: 545-55
 Garabedian & Yamamoto, (1992) *Mol. Biol. Cell* 3: 1245-1257
 Giguere *et al.*, (1986) *Cell* 46: 645-652
 Godowski *et al.*, (1987) *Nature* 325: 365-368
 Goodford, (1985) *J. Med. Chem.* 28: 849-57
 Goodsell & Olsen, (1990) *Proteins* 8: 195-202
 Green & Chambon, (1987) *Nature* 325: 75-78
 Gribskov *et al.*, (1986) *Nucl. Acids. Res.* 14: 6745
 Gruol *et al.*, (1989) *Molec. Endocrinol.* 3: 2119-2127

- Harlow & Lane, (1988) Antibodies: A Laboratory Manual, Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York, United States of America
- Harmon et al., (1979) *J. Cell Physiol.* 98: 267-278
- Hauptman, (1997) *Curr. Opin. Struct. Biol.* 7: 672-80
- 5 Henikoff & Henikoff, (1989) *Proc. Natl. Acad. Sci. U.S.A.* 89: 10915
- Hollenberg & Evans, (1988) *Cell* 55: 899-906
- Hollenberg et al., (1987) *Cell* 49: 39-46
- Hollenberg et al., (1989) *Cancer Res.* 49: 2292s-2294s
- Homo-Delarche, (1984) *Cancer Res.* 44: 431-437
- 10 Janknecht, (1991) *Proc. Natl. Acad. Sci. U.S.A.* 88: 8972-8976
- Jenkins et al., (2001) *Trends Endocrinol. Metab.* 12: 122-126
- Karlin & Altschul, (1993) *Proc. Natl. Acad. Sci. U.S.A.* 90: 5873-5887
- Kelso & Munck, (1984) *J. Immunol.* 133:784-791
- Kralli et al., (1995) *Proc. Natl. Acad. Sci.* 92: 4701-4705
- 15 Kuntz et al., (1992) *J. Mol. Biol.* 161: 269-88
- Kyte & Doolittle, (1982), *J. Mol. Biol.* 157: 105-132
- Lambert, (1997) in Practical Application of Computer-Aided Drug Design, (Charifson, ed.) Marcel-Dekker, New York, New York, United States of America, pp. 243-303
- Lattman, (1985) *Method Enzymol.*, 115: 55-77
- 20 Martin, (1992) *J. Med. Chem.* 35: 2145-54
- Matias et al., (2000) *J. Biol. Chem.* 275:26164-26171
- McConkey et al., (1989) *Arch. Biochem. Biophys.* 269: 365-370
- McPherson, (1982) Preparation and Analysis of Protein Crystals, John Wiley, New York
- McPherson, (1990) *Eur. J. Biochem.* 189:1-23
- 25 McRee, (1992) *J. Mol. Graphics* 10: 44-46
- McRee, (1993) Practical Protein Crystallography, Academic Press, San Diego, California, United States of America
- Miesfeld et al., (1987) *Science* 236:423-427
- Miranker & Karplus, (1991) *Proteins* 11: 29-34
- Navia & Murcko, (1992) *Curr. Opin. Struct. Biol.* 2: 202-10
- 30 Needleman et al., (1970) *J. Mol. Biol.* 48: 443
- Nicholls et al., (1991) *Proteins* 11: 281
- Nimmagadda et al., (1998) *Ann. Allerg. Asthma Im.* 81:35-40
- Nishibata & Itai, (1991) *Tetrahedron* 47: 8985
- Nolte et al., (1998) *Nature* 395:137-43
- 35 Oakley et al., (1996) *J. Biol. Chem.* 271: 9550-9559
- Oberfield et al., (1999) *Proc. Natl. Acad. Sci. U. S. A.* 96(11):6102-6
- Ohara-Nemoto et al., (1990) *J. Steroid Biochem. Molec. Biol.* 37: 481-490
- Oro et al., (1988) *Cell* 55: 1109-1114
- Palmer et al., (2001) *J. Steroid. Biochem. Mol. Biol.* 75:33-42
- 40 Parks et al., (1999) *Science* 284: 1365-1368
- Pearlman et al., (1995) *Comput. Phys. Commun.* 91: 1-41
- Picard & Yamamoto, (1987) *EMBO J.* 6: 3333-3340
- Picard et al., (1990) *Cell Regul.* 1: 291-299
- Rajapandi et al., (2000) *J. Biol. Chem.* 275: 22597-22604
- 45 Rarey et al., (1996) *J. Comput. Aid. Mol. Des.* 10:41-54
- Rossmann (ed.), (1972) The Molecular Replacement Method, Gordon & Breach, New York, New York, United States of America
- Sack et al., (2001) *Proc. Natl. Acad. Sci.* 98:4904-4909
- 50 Sambrook et al., (1989) Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Laboratory, New York, United States of America
- Schwartz et al. (eds.), (1979), Atlas of Protein Sequence and Structure, National Biomedical Research Foundation, pp. 357-358
- Seielstad et al., (1995) *Mol. Endocrinol.* 9: 647-658
- Sheldrick, (1990) *Acta Cryst. A* 46: 467
- 55 Shiau et al., (1998) *Cell* 95: 927-37
- Sladek et al., *Genes Dev.* 4:2353-65
- Smith et al., (1981) *Adv. Appl. Math.* 2:482
- Thompson, (1989) *Cancer Res.* 49: 2259s-2265s

Tucker et al., (1988) *J. Med. Chem.* 31:954
Umesono & Evans, (1989) *Cell* 57: 1139-1146
Van Holde, (1971) *Physical Biochemistry*, Prentice-Hall, New Jersey, pp. 221-39
Voegel et al., (1998) *EMBO J.* 17: 507-519
5 Weber, (1991) *Adv. Protein Chem.* 41:1-36
Weeks et al., (1993) *Acta Cryst. D* 49: 179
Wellner, (1971) *Anal. Chem.* 43: 597
Wetmur & Davidson, (1968) *J. Mol. Biol.* 31: 349-70
Willams & Sigler, (1998) *Nature* 393:392-396
10 Xu et al., (1998) *J. Biol. Chem.* 273: 13918-13924
Yamamoto, (1985) *Ann. Rev. Genet.* 19: 209-252
Yudt & Cidlowski, (2001) *Molec. Endocrinol.* 15: 1093-1103
Yuh & Thompson, (1989) *J. Biol. Chem.* 264: 10904-10910
Zhang et al., (1997) *Nature* 387:206-9
15 Zhou et al., (1998) *Mol. Endocrinol.* 12: 1594-1604
U.S. Patent No. 4,196,265
U.S. Patent No. 4,554,101
U.S. Patent No. 5,260,203
U.S. Patent No. 5,463,564
20 U.S. Patent No. 5,684,151
U.S. Patent No. 5,834,228
U.S. Patent No. 5,872,011
U.S. Patent No. 6,008,033
U.S. Patent No. 6,236,946
25 WO 02/10143
WO 84/03564

TABLE 1

30	STATISTICS OF CRYSTALLOGRAPHIC DATA AND STRUCTURE	
	Crystals	GR/TIF2 in complex with Fluticasone Propionate
	Space Group	P6 ₁
	Resolution (Å)	20.0- 2.5
35	Unique Reflections (N)	28,224
	Completeness (%)	99.7
	I/σ	26.8
	R _{sym} ^a (%)	8.5
40	Refinement Statistics:	
	Resolution (Å)	10.0-2.6
	R factor ^b (%)	24.47
45	R free (%)	27.49
	R.M.S.D.	
	Bond Lengths (Å)	0.016
	R.M.S.D. Bond	
	Angles(degrees)	2.34
50	Number of H ₂ O	145
	Total Non-hydrogen	4589
	Atoms	

R.M.S.D. is the root mean square deviation from ideal geometry.
55 ^aR_{sym}=Σ |avg -I| / Σ I
^bR_{factor}= | F_p - F_{pcalc} | / Σ F_p,
where F_p and F_{pcalc} are observed and calculated structure factors, R_{free} is calculated from a randomly chosen 8% of reflections that never be
used in refinement and R_{factor} is calculated for the remaining 92% of reflections.

TABLE 2

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1	CB	ALA	523	65.188	9.713	-17.288	1.00	138.77	A
2	C	ALA	523	63.798	11.629	-16.450	1.00	138.81	A
3	O	ALA	523	63.723	12.079	-15.303	1.00	139.25	A
4	N	ALA	523	66.269	11.624	-16.161	1.00	138.92	A
5	CA	ALA	523	65.144	11.215	-17.046	1.00	138.73	A
6	N	THR	524	62.743	11.446	-17.237	1.00	138.36	A
7	CA	THR	524	61.387	11.854	-16.883	1.00	137.51	A
8	CB	THR	524	60.369	11.258	-17.876	1.00	137.43	A
9	OG1	THR	524	60.906	11.379	-19.190	1.00	137.90	A
10	CG2	THR	524	59.044	12.033	-17.854	1.00	137.31	A
11	C	THR	524	60.839	11.661	-15.489	1.00	136.92	A
12	O	THR	524	61.408	11.005	-14.628	1.00	137.02	A
13	N	LEU	525	59.703	12.304	-15.311	1.00	136.09	A
14	CA	LEU	525	58.954	12.290	-14.094	1.00	134.94	A
15	CB	LEU	525	59.864	12.306	-12.838	1.00	134.72	A
16	CG	LEU	525	60.146	11.153	-11.810	1.00	134.77	A
17	CD1	LEU	525	58.986	10.507	-11.287	1.00	134.77	A
18	CD2	LEU	525	60.920	10.054	-12.398	1.00	134.85	A
19	C	LEU	525	58.023	13.514	-14.176	1.00	133.93	A
20	O	LEU	525	58.206	14.401	-15.010	1.00	134.00	A
21	N	PRO	526	57.023	13.566	-13.292	1.00	132.74	A
22	CD	PRO	526	55.931	14.501	-13.003	1.00	132.69	A
23	CA	PRO	526	57.030	12.420	-12.404	1.00	131.51	A
24	CB	PRO	526	55.930	12.705	-11.385	1.00	131.91	A
25	CG	PRO	526	55.174	13.816	-11.901	1.00	132.44	A
26	C	PRO	526	57.009	10.986	-12.877	1.00	130.00	A
27	O	PRO	526	57.248	10.597	-14.033	1.00	129.99	A
28	N	GLN	527	56.831	10.220	-11.829	1.00	128.09	A
29	CA	GLN	527	56.837	8.807	-11.797	1.00	125.23	A
30	CB	GLN	527	55.643	8.376	-10.987	1.00	125.24	A
31	CG	GLN	527	55.443	9.354	-9.824	1.00	125.04	A
32	CD	GLN	527	56.752	9.725	-9.106	1.00	124.76	A
33	OE1	GLN	527	57.722	8.964	-9.117	1.00	124.80	A
34	NE2	GLN	527	56.770	10.892	-8.461	1.00	124.17	A
35	C	GLN	527	56.986	8.041	-13.057	1.00	122.94	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
36	O	GLN	527	56.017	7.593	-13.642	1.00	123.03	A
37	N	LEU	528	58.213	7.963	-13.535	1.00	119.79	A
38	CA	LEU	528	58.407	7.079	-14.638	1.00	116.21	A
39	CB	LEU	528	59.246	7.658	-15.761	1.00	116.64	A
40	CG	LEU	528	58.345	7.394	-16.977	1.00	116.96	A
41	CD1	LEU	528	59.130	7.575	-18.243	1.00	117.15	A
42	CD2	LEU	528	57.763	5.970	-16.919	1.00	116.94	A
43	C	LEU	528	59.161	6.052	-13.836	1.00	113.51	A
44	O	LEU	528	59.794	5.149	-14.363	1.00	113.46	A
45	N	THR	529	59.050	6.229	-12.520	1.00	110.03	A
46	CA	THR	529	59.669	5.385	-11.513	1.00	106.14	A
47	CB	THR	529	61.184	5.482	-11.576	1.00	106.80	A
48	OG1	THR	529	61.553	6.661	-12.300	1.00	107.42	A
49	CG2	THR	529	61.748	4.253	-12.268	1.00	107.43	A
50	C	THR	529	59.162	5.870	-10.163	1.00	102.32	A
51	O	THR	529	59.786	6.705	-9.505	1.00	102.18	A
52	N	PRO	530	58.041	5.292	-9.722	1.00	98.65	A
53	CD	PRO	530	57.966	3.889	-10.144	1.00	97.93	A
54	CA	PRO	530	57.228	5.477	-8.520	1.00	96.17	A
55	CB	PRO	530	56.233	4.320	-8.566	1.00	96.64	A
56	CG	PRO	530	56.596	3.514	-9.758	1.00	96.77	A
57	C	PRO	530	57.911	5.556	-7.183	1.00	93.87	A
58	O	PRO	530	58.930	4.922	-6.916	1.00	93.23	A
59	N	THR	531	57.261	6.307	-6.315	1.00	91.25	A
60	CA	THR	531	57.776	6.562	-5.003	1.00	89.02	A
61	CB	THR	531	57.936	8.030	-4.841	1.00	89.18	A
62	OG1	THR	531	56.641	8.646	-4.893	1.00	88.94	A
63	CG2	THR	531	58.762	8.564	-5.981	1.00	88.16	A
64	C	THR	531	56.845	6.079	-3.941	1.00	87.31	A
65	O	THR	531	55.680	5.783	-4.204	1.00	86.50	A
66	N	LEU	532	57.336	6.023	-2.722	1.00	85.91	A
67	CA	LEU	532	56.425	5.574	-1.727	1.00	84.44	A
68	CB	LEU	532	57.077	5.511	-0.355	1.00	83.60	A
69	CG	LEU	532	56.840	4.026	-0.104	1.00	82.34	A
70	CD1	LEU	532	56.814	3.701	1.352	1.00	83.51	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	71	CD2	LEU	532	55.483	3.652	-0.701	1.00	81.89	A
	72	C	LEU	532	55.159	6.426	-1.720	1.00	84.30	A
10	73	O	LEU	532	54.047	5.897	-1.757	1.00	85.02	A
	74	N	VAL	533	55.338	7.742	-1.743	1.00	82.66	A
	75	CA	VAL	533	54.240	8.696	-1.706	1.00	80.63	A
15	76	CB	VAL	533	54.801	10.064	-1.381	1.00	79.39	A
	77	CG1	VAL	533	55.615	10.561	-2.562	1.00	79.10	A
	78	CG2	VAL	533	53.691	11.005	-1.029	1.00	78.78	A
	79	C	VAL	533	53.401	8.825	-2.987	1.00	80.22	A
20	80	O	VAL	533	52.344	9.457	-2.994	1.00	80.48	A
	81	N	SER	534	53.883	8.234	-4.068	1.00	78.78	A
	82	CA	SER	534	53.202	8.309	-5.353	1.00	77.29	A
25	83	CB	SER	534	54.226	8.107	-6.456	1.00	79.18	A
	84	OG	SER	534	53.604	7.680	-7.650	1.00	82.05	A
	85	C	SER	534	52.180	7.214	-5.427	1.00	75.67	A
	86	O	SER	534	51.079	7.364	-5.959	1.00	75.13	A
30	87	N	LEU	535	52.615	6.092	-4.892	1.00	74.52	A
	88	CA	LEU	535	51.854	4.884	-4.835	1.00	73.20	A
	89	CB	LEU	535	52.783	3.790	-4.355	1.00	72.45	A
35	90	CG	LEU	535	52.371	2.441	-4.887	1.00	71.93	A
	91	CD1	LEU	535	51.281	1.873	-4.022	1.00	70.60	A
	92	CD2	LEU	535	51.903	2.610	-6.308	1.00	72.73	A
	93	C	LEU	535	50.730	5.105	-3.851	1.00	73.41	A
40	94	O	LEU	535	49.601	4.640	-4.032	1.00	73.44	A
	95	N	LEU	536	51.055	5.844	-2.804	1.00	73.02	A
	96	CA	LEU	536	50.093	6.137	-1.768	1.00	72.88	A
45	97	CB	LEU	536	50.814	6.850	-0.629	1.00	71.91	A
	98	CG	LEU	536	50.740	6.099	0.706	1.00	69.79	A
	99	CD1	LEU	536	51.084	4.641	0.531	1.00	67.04	A
	100	CD2	LEU	536	51.681	6.752	1.685	1.00	70.08	A
50	101	C	LEU	536	48.929	6.972	-2.299	1.00	72.91	A
	102	O	LEU	536	47.806	6.895	-1.796	1.00	71.27	A
	103	N	GLU	537	49.217	7.738	-3.348	1.00	74.45	A
55	104	CA	GLU	537	48.268	8.637	-3.988	1.00	74.79	A
	105	CB	GLU	537	49.044	9.639	-4.847	1.00	76.31	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
106	CG	GLU	537	48.580	11.065	-4.663	1.00	78.43	A
107	CD	GLU	537	49.645	12.119	-4.966	1.00	80.45	A
108	OE1	GLU	537	50.867	11.850	-4.838	1.00	82.51	A
109	OE2	GLU	537	49.238	13.247	-5.310	1.00	80.91	A
110	C	GLU	537	47.203	7.959	-4.843	1.00	74.83	A
111	O	GLU	537	46.055	8.404	-4.881	1.00	75.79	A
112	N	VAL	538	47.583	6.889	-5.521	1.00	74.12	A
113	CA	VAL	538	46.663	6.190	-6.395	1.00	73.20	A
114	CB	VAL	538	47.423	5.486	-7.509	1.00	72.76	A
115	CG1	VAL	538	48.767	6.147	-7.685	1.00	71.81	A
116	CG2	VAL	538	47.590	4.010	-7.178	1.00	72.29	A
117	C	VAL	538	45.853	5.159	-5.647	1.00	73.07	A
118	O	VAL	538	44.727	4.846	-6.033	1.00	73.83	A
119	N	ILE	539	46.417	4.615	-4.575	1.00	73.33	A
120	CA	ILE	539	45.664	3.608	-3.854	1.00	74.29	A
121	CB	ILE	539	46.586	2.582	-3.130	1.00	73.38	A
122	CG2	ILE	539	47.786	2.259	-4.001	1.00	72.86	A
123	CG1	ILE	539	47.048	3.116	-1.779	1.00	73.08	A
124	CD1	ILE	539	47.600	2.026	-0.885	1.00	72.35	A
125	C	ILE	539	44.676	4.212	-2.865	1.00	74.46	A
126	O	ILE	539	43.901	3.487	-2.251	1.00	73.49	A
127	N	GLU	540	44.691	5.536	-2.725	1.00	76.23	A
128	CA	GLU	540	43.770	6.223	-1.810	1.00	78.11	A
129	CB	GLU	540	44.092	7.730	-1.758	1.00	78.20	A
130	CG	GLU	540	43.208	8.584	-0.829	1.00	79.83	A
131	CD	GLU	540	43.279	8.199	0.649	1.00	80.76	A
132	OE1	GLU	540	44.294	8.501	1.311	1.00	81.61	A
133	OE2	GLU	540	42.309	7.597	1.157	1.00	80.13	A
134	C	GLU	540	42.341	5.984	-2.309	1.00	78.89	A
135	O	GLU	540	42.016	6.288	-3.462	1.00	79.27	A
136	N	PRO	541	41.480	5.397	-1.464	1.00	79.34	A
137	CD	PRO	541	41.713	4.622	-0.233	1.00	79.21	A
138	CA	PRO	541	40.126	5.182	-1.970	1.00	80.63	A
139	CB	PRO	541	39.403	4.466	-0.819	1.00	79.43	A
140	CG	PRO	541	40.335	4.536	0.354	1.00	78.38	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	141	C	PRO	541	39.450	6.469	-2.371	1.00	82.68	A
	142	O	PRO	541	39.811	7.548	-1.892	1.00	82.05	A
10	143	N	GLU	542	38.494	6.370	-3.283	1.00	85.63	A
	144	CA	GLU	542	37.803	7.576	-3.659	1.00	88.82	A
	145	CB	GLU	542	37.681	7.713	-5.182	1.00	90.75	A
15	146	CG	GLU	542	36.797	6.830	-5.997	1.00	93.88	A
	147	CD	GLU	542	36.660	7.477	-7.363	1.00	96.19	A
	148	OE1	GLU	542	37.715	7.811	-7.953	1.00	97.39	A
	149	OE2	GLU	542	35.523	7.687	-7.836	1.00	97.14	A
20	150	C	GLU	542	36.491	7.641	-2.888	1.00	89.50	A
	151	O	GLU	542	35.965	6.619	-2.456	1.00	89.69	A
	152	N	VAL	543	35.994	8.859	-2.684	1.00	90.04	A
25	153	CA	VAL	543	34.820	9.119	-1.843	1.00	90.75	A
	154	CB	VAL	543	34.644	10.627	-1.691	1.00	91.20	A
	155	CG1	VAL	543	33.946	10.911	-0.379	1.00	90.59	A
	156	CG2	VAL	543	36.004	11.325	-1.750	1.00	90.81	A
30	157	C	VAL	543	33.417	8.509	-2.014	1.00	91.22	A
	158	O	VAL	543	32.778	8.651	-3.057	1.00	91.07	A
	159	N	LEU	544	32.926	7.891	-0.936	1.00	91.90	A
35	160	CA	LEU	544	31.607	7.231	-0.896	1.00	93.16	A
	161	CB	LEU	544	31.695	5.928	-0.076	1.00	93.10	A
	162	CG	LEU	544	32.356	4.691	-0.694	1.00	93.35	A
	163	CD1	LEU	544	31.473	3.432	-0.558	1.00	93.98	A
40	164	CD2	LEU	544	32.607	4.994	-2.153	1.00	93.53	A
	165	C	LEU	544	30.382	8.011	-0.378	1.00	94.32	A
	166	O	LEU	544	30.268	8.268	0.826	1.00	94.86	A
45	167	N	TYR	545	29.456	8.340	-1.289	1.00	94.95	A
	168	CA	TYR	545	28.207	9.051	-0.955	1.00	94.71	A
	169	CB	TYR	545	27.465	9.466	-2.233	1.00	96.89	A
	170	CG	TYR	545	28.215	10.538	-2.990	1.00	99.74	A
50	171	CD1	TYR	545	29.253	10.210	-3.860	1.00	101.09	A
	172	CE1	TYR	545	30.049	11.206	-4.440	1.00	102.49	A
	173	CD2	TYR	545	27.978	11.887	-2.732	1.00	101.22	A
55	174	CE2	TYR	545	28.764	12.886	-3.299	1.00	102.50	A
	175	CZ	TYR	545	29.800	12.540	-4.151	1.00	103.07	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
176	OH	TYR	545	30.613	13.525	-4.675	1.00	103.71	A
177	C	TYR	545	27.346	8.126	-0.100	1.00	93.35	A
178	O	TYR	545	27.512	6.914	-0.165	1.00	92.28	A
179	N	ALA	546	26.415	8.678	0.677	1.00	92.46	A
180	CA	ALA	546	25.627	7.836	1.583	1.00	91.68	A
181	CB	ALA	546	25.512	8.536	2.941	1.00	91.47	A
182	C	ALA	546	24.259	7.289	1.195	1.00	90.98	A
183	O	ALA	546	23.712	6.466	1.930	1.00	91.08	A
184	N	GLY	547	23.696	7.714	0.069	1.00	90.37	A
185	CA	GLY	547	22.380	7.214	-0.302	1.00	89.38	A
186	C	GLY	547	21.359	7.574	0.767	1.00	88.66	A
187	O	GLY	547	20.486	6.780	1.119	1.00	88.42	A
188	N	TYR	548	21.480	8.778	1.298	1.00	88.15	A
189	CA	TYR	548	20.574	9.246	2.327	1.00	86.95	A
190	CB	TYR	548	21.255	10.322	3.156	1.00	85.67	A
191	CG	TYR	548	20.496	10.787	4.372	1.00	84.73	A
192	CD1	TYR	548	20.476	10.024	5.538	1.00	84.74	A
193	CE1	TYR	548	19.896	10.510	6.706	1.00	84.64	A
194	CD2	TYR	548	19.892	12.043	4.396	1.00	83.83	A
195	CE2	TYR	548	19.310	12.534	5.553	1.00	84.34	A
196	CZ	TYR	548	19.321	11.763	6.707	1.00	84.86	A
197	OH	TYR	548	18.801	12.254	7.882	1.00	86.53	A
198	C	TYR	548	19.379	9.840	1.624	1.00	87.42	A
199	O	TYR	548	19.469	10.266	0.474	1.00	87.52	A
200	N	ASP	549	18.247	9.865	2.300	1.00	88.18	A
201	CA	ASP	549	17.071	10.438	1.694	1.00	88.70	A
202	CB	ASP	549	15.908	9.461	1.770	1.00	90.10	A
203	CG	ASP	549	14.632	10.070	1.281	1.00	91.67	A
204	OD1	ASP	549	14.725	10.951	0.404	1.00	94.32	A
205	OD2	ASP	549	13.552	9.676	1.763	1.00	91.48	A
206	C	ASP	549	16.744	11.720	2.433	1.00	88.75	A
207	O	ASP	549	16.139	11.697	3.494	1.00	88.40	A
208	N	SER	550	17.150	12.851	1.876	1.00	89.12	A
209	CA	SER	550	16.888	14.115	2.544	1.00	89.61	A
210	CB	SER	550	18.044	15.106	2.319	1.00	90.04	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	211	OG	SER	550	18.345	15.283	0.947	1.00	90.73	A
	212	C	SER	550	15.564	14.714	2.123	1.00	89.18	A
10	213	O	SER	550	15.241	15.849	2.479	1.00	89.03	A
	214	N	SER	551	14.791	13.964	1.357	1.00	88.84	A
	215	CA	SER	551	13.493	14.483	0.995	1.00	89.26	A
15	216	CB	SER	551	12.878	13.704	-0.168	1.00	89.54	A
	217	OG	SER	551	13.113	12.324	-0.037	1.00	91.73	A
	218	C	SER	551	12.634	14.390	2.256	1.00	88.19	A
	219	O	SER	551	11.603	15.030	2.341	1.00	88.72	A
20	220	N	VAL	552	13.058	13.610	3.250	1.00	87.55	A
	221	CA	VAL	552	12.284	13.527	4.495	1.00	87.25	A
	222	CB	VAL	552	11.830	12.070	4.820	1.00	87.97	A
25	223	CG1	VAL	552	11.975	11.175	3.599	1.00	87.37	A
	224	CG2	VAL	552	12.606	11.529	6.003	1.00	87.92	A
	225	C	VAL	552	13.094	14.092	5.670	1.00	86.73	A
	226	O	VAL	552	14.326	14.022	5.676	1.00	86.64	A
30	227	N	PRO	553	12.410	14.634	6.696	1.00	86.61	A
	228	CD	PRO	553	10.956	14.803	6.833	1.00	86.60	A
	229	CA	PRO	553	13.114	15.213	7.850	1.00	87.41	A
35	230	CB	PRO	553	12.014	15.962	8.591	1.00	87.09	A
	231	CG	PRO	553	10.807	15.185	8.288	1.00	87.29	A
	232	C	PRO	553	13.975	14.371	8.786	1.00	87.77	A
	233	O	PRO	553	13.570	13.322	9.289	1.00	88.30	A
40	234	N	ASP	554	15.171	14.905	9.019	1.00	87.98	A
	235	CA	ASP	554	16.184	14.298	9.868	1.00	88.66	A
	236	CB	ASP	554	17.364	15.258	10.095	1.00	88.19	A
45	237	CG	ASP	554	17.900	15.894	8.820	1.00	88.24	A
	238	OD1	ASP	554	17.439	15.598	7.695	1.00	88.21	A
	239	OD2	ASP	554	18.817	16.722	8.975	1.00	88.62	A
	240	C	ASP	554	15.693	13.903	11.254	1.00	89.18	A
50	241	O	ASP	554	14.574	14.205	11.670	1.00	89.35	A
	242	N	SER	555	16.592	13.245	11.972	1.00	89.93	A
	243	CA	SER	555	16.379	12.799	13.331	1.00	90.27	A
55	244	CB	SER	555	15.277	11.750	13.419	1.00	90.19	A
	245	OG	SER	555	15.647	10.558	12.754	1.00	89.00	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
246	C	SER	555	17.715	12.181	13.672	1.00	91.27	A
247	O	SER	555	18.445	11.746	12.780	1.00	90.85	A
248	N	THR	556	18.041	12.149	14.950	1.00	92.81	A
249	CA	THR	556	19.317	11.597	15.357	1.00	94.66	A
250	CB	THR	556	19.533	11.760	16.870	1.00	95.26	A
251	OG1	THR	556	20.067	13.062	17.143	1.00	95.78	A
252	CG2	THR	556	20.489	10.713	17.379	1.00	95.54	A
253	C	THR	556	19.557	10.141	14.977	1.00	95.12	A
254	O	THR	556	20.654	9.819	14.514	1.00	94.58	A
255	N	TRP	557	18.561	9.266	15.168	1.00	96.53	A
256	CA	TRP	557	18.725	7.837	14.850	1.00	97.64	A
257	CB	TRP	557	17.556	6.977	15.403	1.00	100.93	A
258	CG	TRP	557	16.527	6.440	14.377	1.00	105.32	A
259	CD2	TRP	557	16.552	5.170	13.683	1.00	106.95	A
260	CE2	TRP	557	15.425	5.135	12.826	1.00	107.45	A
261	CE3	TRP	557	17.409	4.057	13.709	1.00	107.83	A
262	CD1	TRP	557	15.417	7.096	13.913	1.00	106.74	A
263	NE1	TRP	557	14.754	6.320	12.983	1.00	107.65	A
264	CZ2	TRP	557	15.142	4.040	11.988	1.00	107.79	A
265	CZ3	TRP	557	17.123	2.963	12.875	1.00	108.24	A
266	CH2	TRP	557	15.996	2.967	12.032	1.00	107.96	A
267	C	TRP	557	18.884	7.612	13.355	1.00	96.37	A
268	O	TRP	557	19.697	6.803	12.916	1.00	96.21	A
269	N	ARG	558	18.117	8.351	12.580	1.00	95.03	A
270	CA	ARG	558	18.164	8.243	11.139	1.00	93.86	A
271	CB	ARG	558	17.054	9.068	10.566	1.00	93.78	A
272	CG	ARG	558	16.719	8.624	9.224	1.00	94.44	A
273	CD	ARG	558	15.975	9.679	8.550	1.00	94.58	A
274	NE	ARG	558	16.253	9.641	7.134	1.00	95.72	A
275	CZ	ARG	558	16.025	10.672	6.351	1.00	96.79	A
276	NH1	ARG	558	15.513	11.775	6.873	1.00	98.36	A
277	NH2	ARG	558	16.334	10.612	5.077	1.00	96.49	A
278	C	ARG	558	19.461	8.773	10.561	1.00	93.25	A
279	O	ARG	558	19.887	8.406	9.467	1.00	93.99	A
280	N	ILE	559	20.070	9.683	11.291	1.00	91.60	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	281	CA	ILE	559	21.280	10.294	10.812	1.00	89.71	A
	282	CB	ILE	559	21.492	11.590	11.494	1.00	88.91	A
10	283	CG2	ILE	559	22.970	11.817	11.655	1.00	87.58	A
	284	CG1	ILE	559	20.833	12.699	10.697	1.00	88.10	A
	285	CD1	ILE	559	21.767	13.323	9.711	1.00	86.84	A
15	286	C	ILE	559	22.514	9.481	11.063	1.00	89.28	A
	287	O	ILE	559	23.505	9.565	10.329	1.00	88.46	A
	288	N	MET	560	22.486	8.742	12.149	1.00	88.75	A
	289	CA	MET	560	23.651	7.976	12.426	1.00	88.01	A
20	290	CB	MET	560	24.089	8.152	13.864	1.00	87.86	A
	291	CG	MET	560	22.989	8.134	14.830	1.00	87.31	A
	292	SD	MET	560	23.689	8.279	16.446	1.00	90.24	A
25	293	CE	MET	560	22.239	8.344	17.386	1.00	88.07	A
	294	C	MET	560	23.471	6.542	12.062	1.00	87.94	A
	295	O	MET	560	24.281	5.703	12.418	1.00	89.01	A
	296	N	THR	561	22.401	6.202	11.378	1.00	87.34	A
30	297	CA	THR	561	22.443	4.835	10.977	1.00	86.95	A
	298	CB	THR	561	21.093	4.175	10.912	1.00	87.31	A
	299	OG1	THR	561	20.928	3.364	12.087	1.00	87.10	A
35	300	CG2	THR	561	21.020	3.289	9.681	1.00	87.30	A
	301	C	THR	561	23.112	4.874	9.612	1.00	86.05	A
	302	O	THR	561	24.027	4.104	9.345	1.00	86.32	A
	303	N	THR	562	22.686	5.803	8.762	1.00	85.38	A
40	304	CA	THR	562	23.254	5.931	7.431	1.00	85.67	A
	305	CB	THR	562	22.661	7.175	6.763	1.00	85.65	A
	306	OG1	THR	562	21.230	7.079	6.820	1.00	85.77	A
45	307	CG2	THR	562	23.098	7.282	5.312	1.00	85.39	A
	308	C	THR	562	24.774	6.055	7.544	1.00	85.77	A
	309	O	THR	562	25.539	5.598	6.665	1.00	86.58	A
	310	N	LEU	563	25.190	6.642	8.661	1.00	84.92	A
50	311	CA	LEU	563	26.579	6.904	8.938	1.00	82.98	A
	312	CB	LEU	563	26.574	7.878	10.095	1.00	82.31	A
	313	CG	LEU	563	27.148	9.271	9.752	1.00	81.13	A
55	314	CD1	LEU	563	26.867	9.649	8.298	1.00	79.57	A
	315	CD2	LEU	563	26.558	10.334	10.667	1.00	79.28	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
316	C	LEU	563	27.298	5.591	9.252	1.00	82.41	A
317	O	LEU	563	28.455	5.334	8.868	1.00	82.20	A
318	N	ASN	564	26.593	4.751	9.975	1.00	81.88	A
319	CA	ASN	564	27.155	3.478	10.274	1.00	81.91	A
320	CB	ASN	564	26.246	2.805	11.249	1.00	81.34	A
321	CG	ASN	564	26.562	3.217	12.637	1.00	81.57	A
322	OD1	ASN	564	26.978	4.352	12.886	1.00	81.79	A
323	ND2	ASN	564	26.387	2.297	13.559	1.00	82.16	A
324	C	ASN	564	27.242	2.755	8.952	1.00	81.96	A
325	O	ASN	564	28.304	2.329	8.539	1.00	82.86	A
326	N	MET	565	26.113	2.617	8.281	1.00	81.73	A
327	CA	MET	565	26.088	1.995	6.978	1.00	81.37	A
328	CB	MET	565	24.744	2.265	6.354	1.00	82.20	A
329	CG	MET	565	23.649	1.696	7.190	1.00	83.63	A
330	SD	MET	565	23.641	-0.044	6.893	1.00	87.40	A
331	CE	MET	565	23.455	-0.696	8.521	1.00	85.88	A
332	C	MET	565	27.200	2.581	6.113	1.00	80.49	A
333	O	MET	565	27.821	1.862	5.333	1.00	81.60	A
334	N	LEU	566	27.450	3.884	6.224	1.00	78.75	A
335	CA	LEU	566	28.545	4.438	5.437	1.00	77.41	A
336	CB	LEU	566	28.605	5.973	5.503	1.00	76.81	A
337	CG	LEU	566	29.358	6.582	4.305	1.00	76.68	A
338	CD1	LEU	566	29.976	7.929	4.627	1.00	75.40	A
339	CD2	LEU	566	30.456	5.629	3.906	1.00	78.41	A
340	C	LEU	566	29.786	3.827	6.097	1.00	77.16	A
341	O	LEU	566	30.806	3.581	5.453	1.00	75.61	A
342	N	GLY	567	29.669	3.566	7.396	1.00	77.62	A
343	CA	GLY	567	30.752	2.961	8.154	1.00	77.48	A
344	C	GLY	567	31.245	1.671	7.527	1.00	78.30	A
345	O	GLY	567	32.411	1.585	7.145	1.00	78.23	A
346	N	GLY	568	30.371	0.671	7.410	1.00	78.02	A
347	CA	GLY	568	30.776	-0.588	6.815	1.00	77.12	A
348	C	GLY	568	31.491	-0.437	5.479	1.00	76.89	A
349	O	GLY	568	32.611	-0.917	5.312	1.00	78.89	A
350	N	ARG	569	30.860	0.234	4.525	1.00	75.25	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	351	CA	ARG	569	31.463	0.391	3.212	1.00	75.08	A
	352	CB	ARG	569	30.550	1.219	2.304	1.00	76.25	A
10	353	CG	ARG	569	29.293	0.458	1.878	1.00	77.82	A
	354	CD	ARG	569	28.574	1.141	0.734	1.00	78.35	A
	355	NE	ARG	569	28.004	2.413	1.141	1.00	80.79	A
15	356	CZ	ARG	569	28.127	3.537	0.439	1.00	82.46	A
	357	NH1	ARG	569	28.808	3.533	-0.698	1.00	82.95	A
	358	NH2	ARG	569	27.573	4.660	0.871	1.00	82.74	A
	359	C	ARG	569	32.859	0.990	3.251	1.00	74.49	A
20	360	O	ARG	569	33.778	0.496	2.595	1.00	74.53	A
	361	N	GLN	570	33.016	2.056	4.028	1.00	73.65	A
	362	CA	GLN	570	34.304	2.722	4.155	1.00	71.97	A
25	363	CB	GLN	570	34.160	3.957	5.032	1.00	72.89	A
	364	CG	GLN	570	34.204	5.270	4.286	1.00	72.15	A
	365	CD	GLN	570	33.699	6.384	5.147	1.00	71.88	A
	366	OE1	GLN	570	33.539	7.513	4.692	1.00	72.77	A
30	367	NE2	GLN	570	33.434	6.074	6.412	1.00	71.54	A
	368	C	GLN	570	35.344	1.797	4.762	1.00	70.46	A
	369	O	GLN	570	36.477	1.728	4.286	1.00	70.24	A
35	370	N	VAL	571	34.959	1.100	5.824	1.00	68.82	A
	371	CA	VAL	571	35.850	0.165	6.499	1.00	68.22	A
	372	CB	VAL	571	35.133	-0.539	7.669	1.00	68.99	A
	373	CG1	VAL	571	35.836	-1.845	8.004	1.00	66.89	A
40	374	CG2	VAL	571	35.114	0.371	8.886	1.00	69.13	A
	375	C	VAL	571	36.358	-0.887	5.525	1.00	67.65	A
	376	O	VAL	571	37.553	-1.197	5.492	1.00	67.31	A
45	377	N	ILE	572	35.436	-1.443	4.742	1.00	67.57	A
	378	CA	ILE	572	35.784	-2.451	3.747	1.00	67.90	A
	379	CB	ILE	572	34.517	-2.964	3.017	1.00	68.96	A
	380	CG2	ILE	572	34.870	-3.480	1.617	1.00	68.69	A
50	381	CG1	ILE	572	33.863	-4.063	3.870	1.00	69.67	A
	382	CD1	ILE	572	32.347	-4.003	3.945	1.00	68.89	A
	383	C	ILE	572	36.760	-1.832	2.768	1.00	67.12	A
55	384	O	ILE	572	37.777	-2.428	2.448	1.00	68.93	A
	385	N	ALA	573	36.464	-0.630	2.308	1.00	66.15	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
386	CA	ALA	573	37.356	0.054	1.383	1.00	66.46	A
387	CB	ALA	573	36.840	1.478	1.108	1.00	65.79	A
388	C	ALA	573	38.771	0.116	1.967	1.00	66.93	A
389	O	ALA	573	39.766	-0.012	1.238	1.00	65.81	A
390	N	ALA	574	38.843	0.312	3.287	1.00	67.23	A
391	CA	ALA	574	40.110	0.419	4.014	1.00	67.61	A
392	CB	ALA	574	39.846	0.728	5.486	1.00	67.60	A
393	C	ALA	574	40.942	-0.847	3.894	1.00	67.98	A
394	O	ALA	574	42.168	-0.789	3.797	1.00	67.69	A
395	N	VAL	575	40.265	-1.992	3.912	1.00	67.17	A
396	CA	VAL	575	40.937	-3.273	3.792	1.00	66.42	A
397	CB	VAL	575	39.946	-4.428	3.976	1.00	65.00	A
398	CG1	VAL	575	40.670	-5.734	3.877	1.00	64.48	A
399	CG2	VAL	575	39.261	-4.314	5.314	1.00	64.37	A
400	C	VAL	575	41.645	-3.404	2.428	1.00	66.62	A
401	O	VAL	575	42.841	-3.686	2.380	1.00	66.81	A
402	N	LYS	576	40.918	-3.183	1.329	1.00	66.28	A
403	CA	LYS	576	41.495	-3.282	-0.024	1.00	66.17	A
404	CB	LYS	576	40.403	-3.082	-1.076	1.00	67.84	A
405	CG	LYS	576	40.917	-2.933	-2.521	1.00	70.31	A
406	CD	LYS	576	39.757	-2.724	-3.500	1.00	72.81	A
407	CE	LYS	576	38.675	-3.803	-3.306	1.00	74.86	A
408	NZ	LYS	576	37.379	-3.492	-4.002	1.00	76.42	A
409	C	LYS	576	42.601	-2.249	-0.253	1.00	65.27	A
410	O	LYS	576	43.366	-2.322	-1.221	1.00	66.35	A
411	N	TRP	577	42.652	-1.283	0.652	1.00	63.60	A
412	CA	TRP	577	43.617	-0.188	0.636	1.00	60.50	A
413	CB	TRP	577	42.988	1.044	1.280	1.00	57.29	A
414	CG	TRP	577	43.969	2.074	1.708	1.00	52.50	A
415	CD2	TRP	577	44.414	2.330	3.042	1.00	50.81	A
416	CE2	TRP	577	45.370	3.360	2.971	1.00	50.82	A
417	CE3	TRP	577	44.113	1.769	4.293	1.00	49.45	A
418	CD1	TRP	577	44.642	2.943	0.904	1.00	51.34	A
419	NE1	TRP	577	45.484	3.721	1.654	1.00	50.82	A
420	CZ2	TRP	577	46.011	3.873	4.105	1.00	50.90	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	421	CZ3	TRP	577	44.754	2.274	5.421	1.00	49.27	A
	422	CH2	TRP	577	45.697	3.309	5.318	1.00	49.59	A
10	423	C	TRP	577	44.842	-0.583	1.437	1.00	60.60	A
	424	O	TRP	577	45.975	-0.357	1.018	1.00	59.49	A
	425	N	ALA	578	44.591	-1.143	2.617	1.00	61.86	A
15	426	CA	ALA	578	45.657	-1.570	3.507	1.00	63.00	A
	427	CB	ALA	578	45.073	-2.239	4.745	1.00	61.78	A
	428	C	ALA	578	46.541	-2.546	2.759	1.00	64.13	A
	429	O	ALA	578	47.762	-2.444	2.791	1.00	65.39	A
20	430	N	LYS	579	45.901	-3.480	2.065	1.00	64.92	A
	431	CA	LYS	579	46.608	-4.491	1.308	1.00	64.28	A
	432	CB	LYS	579	45.612	-5.540	0.792	1.00	64.80	A
25	433	CG	LYS	579	44.584	-6.000	1.845	1.00	65.52	A
	434	CD	LYS	579	43.721	-7.234	1.436	1.00	65.27	A
	435	CE	LYS	579	43.635	-7.474	-0.085	1.00	65.83	A
	436	NZ	LYS	579	42.891	-8.722	-0.466	1.00	66.54	A
30	437	C	LYS	579	47.427	-3.916	0.150	1.00	64.31	A
	438	O	LYS	579	48.215	-4.634	-0.447	1.00	66.40	A
	439	N	ALA	580	47.268	-2.637	-0.180	1.00	63.18	A
35	440	CA	ALA	580	48.057	-2.074	-1.278	1.00	63.23	A
	441	CB	ALA	580	47.194	-1.179	-2.159	1.00	63.30	A
	442	C	ALA	580	49.260	-1.291	-0.765	1.00	63.73	A
	443	O	ALA	580	50.146	-0.917	-1.542	1.00	63.06	A
40	444	N	ILE	581	49.273	-1.032	0.543	1.00	64.21	A
	445	CA	ILE	581	50.377	-0.316	1.172	1.00	64.66	A
	446	CB	ILE	581	50.115	-0.041	2.670	1.00	63.87	A
45	447	CG2	ILE	581	51.358	0.554	3.325	1.00	62.27	A
	448	CG1	ILE	581	48.940	0.927	2.812	1.00	62.68	A
	449	CD1	ILE	581	47.956	0.530	3.881	1.00	63.04	A
	450	C	ILE	581	51.552	-1.258	1.035	1.00	66.30	A
50	451	O	ILE	581	51.620	-2.304	1.689	1.00	66.21	A
	452	N	PRO	582	52.480	-0.923	0.142	1.00	67.08	A
	453	CD	PRO	582	52.523	0.254	-0.741	1.00	67.75	A
55	454	CA	PRO	582	53.637	-1.791	-0.037	1.00	68.22	A
	455	CB	PRO	582	54.645	-0.891	-0.770	1.00	68.28	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
456	CG	PRO	582	53.981	0.516	-0.825	1.00	68.57	A
457	C	PRO	582	54.154	-2.320	1.307	1.00	69.73	A
458	O	PRO	582	54.501	-1.537	2.192	1.00	70.65	A
459	N	GLY	583	54.167	-3.641	1.471	1.00	71.35	A
460	CA	GLY	583	54.663	-4.223	2.709	1.00	72.71	A
461	C	GLY	583	53.642	-4.649	3.749	1.00	74.07	A
462	O	GLY	583	53.910	-5.513	4.584	1.00	74.51	A
463	N	PHE	584	52.461	-4.058	3.728	1.00	74.52	A
464	CA	PHE	584	51.485	-4.449	4.716	1.00	74.52	A
465	CB	PHE	584	50.236	-3.586	4.614	1.00	69.69	A
466	CG	PHE	584	49.161	-3.994	5.563	1.00	64.19	A
467	CD1	PHE	584	49.244	-3.660	6.910	1.00	62.21	A
468	CD2	PHE	584	48.078	-4.729	5.115	1.00	61.91	A
469	CE1	PHE	584	48.268	-4.070	7.809	1.00	60.54	A
470	CE2	PHE	584	47.091	-5.147	6.004	1.00	61.98	A
471	CZ	PHE	584	47.180	-4.811	7.354	1.00	60.81	A
472	C	PHE	584	51.089	-5.915	4.565	1.00	77.99	A
473	O	PHE	584	50.806	-6.590	5.566	1.00	78.31	A
474	N	ARG	585	51.066	-6.429	3.337	1.00	80.71	A
475	CA	ARG	585	50.634	-7.812	3.215	1.00	82.98	A
476	CB	ARG	585	49.729	-8.017	1.993	1.00	83.84	A
477	CG	ARG	585	50.239	-7.765	0.590	1.00	86.72	A
478	CD	ARG	585	49.051	-8.111	-0.318	1.00	89.26	A
479	NE	ARG	585	48.267	-9.140	0.371	1.00	92.25	A
480	CZ	ARG	585	47.235	-9.818	-0.119	1.00	93.54	A
481	NH1	ARG	585	46.797	-9.610	-1.359	1.00	94.06	A
482	NH2	ARG	585	46.652	-10.737	0.641	1.00	93.54	A
483	C	ARG	585	51.662	-8.917	3.324	1.00	83.93	A
484	O	ARG	585	51.379	-10.069	3.003	1.00	84.40	A
485	N	ASN	586	52.845	-8.573	3.802	1.00	85.01	A
486	CA	ASN	586	53.871	-9.570	4.022	1.00	85.88	A
487	CB	ASN	586	55.231	-9.061	3.564	1.00	86.01	A
488	CG	ASN	586	55.328	-8.972	2.059	1.00	86.96	A
489	OD1	ASN	586	56.236	-8.339	1.522	1.00	88.16	A
490	ND2	ASN	586	54.388	-9.613	1.363	1.00	86.48	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	491	C	ASN	586	53.846	-9.776	5.518	1.00	86.24	A
	492	O	ASN	586	54.624	-10.539	6.077	1.00	87.32	A
10	493	N	LEU	587	52.932	-9.071	6.169	1.00	86.65	A
	494	CA	LEU	587	52.792	-9.198	7.600	1.00	87.77	A
	495	CB	LEU	587	52.088	-7.970	8.188	1.00	87.74	A
15	496	CG	LEU	587	52.935	-6.697	8.210	1.00	86.52	A
	497	CD1	LEU	587	52.116	-5.534	8.724	1.00	86.30	A
	498	CD2	LEU	587	54.145	-6.924	9.095	1.00	86.53	A
	499	C	LEU	587	51.979	-10.450	7.850	1.00	88.42	A
20	500	O	LEU	587	51.260	-10.930	6.968	1.00	87.25	A
	501	N	HIS	588	52.108	-10.989	9.053	1.00	89.97	A
	502	CA	HIS	588	51.378	-12.191	9.390	1.00	91.55	A
25	503	CB	HIS	588	51.642	-12.574	10.835	1.00	93.32	A
	504	CG	HIS	588	51.068	-13.911	11.192	1.00	95.30	A
	505	CD2	HIS	588	50.156	-14.245	12.137	1.00	95.82	A
	506	ND1	HIS	588	51.401	-15.047	10.527	1.00	96.00	A
30	507	CE1	HIS	588	50.715	-16.075	11.050	1.00	96.43	A
	508	NE2	HIS	588	49.967	-15.608	12.013	1.00	96.43	A
	509	C	HIS	588	49.887	-11.952	9.184	1.00	91.17	A
35	510	O	HIS	588	49.297	-11.142	9.893	1.00	91.33	A
	511	N	LEU	589	49.284	-12.651	8.221	1.00	89.87	A
	512	CA	LEU	589	47.860	-12.477	7.945	1.00	88.11	A
	513	CB	LEU	589	47.284	-13.700	7.221	1.00	88.40	A
40	514	CG	LEU	589	45.765	-13.669	6.969	1.00	88.28	A
	515	CD1	LEU	589	45.400	-14.733	5.962	1.00	88.56	A
	516	CD2	LEU	589	44.979	-13.904	8.259	1.00	88.39	A
45	517	C	LEU	589	47.047	-12.209	9.208	1.00	87.37	A
	518	O	LEU	589	45.969	-11.624	9.127	1.00	86.71	A
	519	N	ASP	590	47.541	-12.642	10.363	1.00	86.54	A
	520	CA	ASP	590	46.833	-12.406	11.625	1.00	85.87	A
50	521	CB	ASP	590	47.294	-13.340	12.734	1.00	86.86	A
	522	CG	ASP	590	46.610	-14.679	12.702	1.00	87.52	A
	523	OD1	ASP	590	45.526	-14.809	12.090	1.00	87.78	A
55	524	OD2	ASP	590	47.167	-15.605	13.323	1.00	87.71	A
	525	C	ASP	590	47.067	-11.002	12.120	1.00	84.92	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	526	O	ASP	590	46.244	-10.458	12.849	1.00	84.94	A
	527	N	ASP	591	48.230	-10.454	11.769	1.00	84.52	A
10	528	CA	ASP	591	48.620	-9.091	12.130	1.00	83.62	A
	529	CB	ASP	591	50.107	-8.838	11.850	1.00	84.12	A
	530	CG	ASP	591	51.022	-9.693	12.697	1.00	84.28	A
	531	OD1	ASP	591	50.727	-9.862	13.899	1.00	84.06	A
15	532	OD2	ASP	591	52.042	-10.183	12.160	1.00	83.73	A
	533	C	ASP	591	47.808	-8.185	11.229	1.00	82.14	A
	534	O	ASP	591	47.205	-7.207	11.669	1.00	81.59	A
20	535	N	GLN	592	47.815	-8.529	9.946	1.00	80.47	A
	536	CA	GLN	592	47.067	-7.782	8.969	1.00	78.87	A
	537	CB	GLN	592	46.947	-8.594	7.690	1.00	77.24	A
25	538	CG	GLN	592	48.091	-8.281	6.782	1.00	76.69	A
	539	CD	GLN	592	48.068	-9.036	5.487	1.00	76.67	A
	540	OE1	GLN	592	47.017	-9.193	4.855	1.00	76.15	A
	541	NE2	GLN	592	49.241	-9.495	5.059	1.00	75.91	A
30	542	C	GLN	592	45.706	-7.450	9.538	1.00	78.83	A
	543	O	GLN	592	45.148	-6.390	9.245	1.00	79.67	A
	544	N	MET	593	45.212	-8.347	10.393	1.00	78.36	A
35	545	CA	MET	593	43.912	-8.231	11.058	1.00	78.31	A
	546	CB	MET	593	43.275	-9.615	11.244	1.00	79.96	A
	547	CG	MET	593	42.329	-10.103	10.149	1.00	82.51	A
	548	SD	MET	593	41.604	-11.744	10.579	1.00	86.38	A
40	549	CE	MET	593	39.882	-11.316	10.995	1.00	84.03	A
	550	C	MET	593	43.900	-7.547	12.428	1.00	77.60	A
	551	O	MET	593	42.843	-7.081	12.859	1.00	77.34	A
45	552	N	THR	594	45.020	-7.507	13.145	1.00	76.82	A
	553	CA	THR	594	44.984	-6.861	14.458	1.00	76.93	A
	554	CB	THR	594	46.140	-7.311	15.391	1.00	77.94	A
	555	OG1	THR	594	46.650	-8.574	14.956	1.00	78.86	A
50	556	CG2	THR	594	45.627	-7.462	16.828	1.00	77.65	A
	557	C	THR	594	45.098	-5.365	14.225	1.00	76.19	A
	558	O	THR	594	44.451	-4.551	14.896	1.00	75.57	A
55	559	N	LEU	595	45.936	-5.021	13.252	1.00	74.76	A
	560	CA	LEU	595	46.147	-3.637	12.882	1.00	72.91	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	561	CB	LEU	595	47.243	-3.554	11.804	1.00	70.46	A
	562	CG	LEU	595	48.681	-3.258	12.261	1.00	67.61	A
10	563	CD1	LEU	595	48.841	-3.596	13.722	1.00	66.68	A
	564	CD2	LEU	595	49.676	-4.028	11.409	1.00	66.99	A
	565	C	LEU	595	44.820	-3.030	12.400	1.00	72.82	A
15	566	O	LEU	595	44.428	-1.966	12.874	1.00	73.34	A
	567	N	LEU	596	44.103	-3.706	11.505	1.00	71.86	A
	568	CA	LEU	596	42.837	-3.154	11.025	1.00	71.08	A
	569	CB	LEU	596	42.307	-3.985	9.868	1.00	67.81	A
20	570	CG	LEU	596	42.995	-3.546	8.584	1.00	65.63	A
	571	CD1	LEU	596	42.589	-4.452	7.451	1.00	65.47	A
	572	CD2	LEU	596	42.625	-2.111	8.286	1.00	64.45	A
25	573	C	LEU	596	41.751	-2.993	12.083	1.00	72.89	A
	574	O	LEU	596	40.990	-2.023	12.061	1.00	72.60	A
	575	N	GLN	597	41.685	-3.940	13.014	1.00	75.30	A
	576	CA	GLN	597	40.688	-3.913	14.080	1.00	77.33	A
30	577	CB	GLN	597	40.550	-5.284	14.700	1.00	79.16	A
	578	CG	GLN	597	39.994	-6.316	13.777	1.00	82.61	A
	579	CD	GLN	597	40.095	-7.697	14.372	1.00	84.85	A
35	580	OE1	GLN	597	39.459	-8.633	13.890	1.00	85.84	A
	581	NE2	GLN	597	40.908	-7.838	15.420	1.00	85.44	A
	582	C	GLN	597	41.068	-2.959	15.177	1.00	77.62	A
	583	O	GLN	597	40.239	-2.546	15.991	1.00	77.11	A
40	584	N	TYR	598	42.335	-2.626	15.233	1.00	78.31	A
	585	CA	TYR	598	42.748	-1.717	16.265	1.00	79.61	A
	586	CB	TYR	598	44.192	-1.982	16.624	1.00	82.08	A
45	587	CG	TYR	598	44.386	-3.073	17.637	1.00	84.90	A
	588	CD1	TYR	598	43.519	-4.168	17.717	1.00	85.68	A
	589	CE1	TYR	598	43.735	-5.174	18.653	1.00	86.83	A
	590	CD2	TYR	598	45.457	-3.014	18.504	1.00	86.14	A
50	591	CE2	TYR	598	45.684	-4.000	19.426	1.00	87.17	A
	592	CZ	TYR	598	44.831	-5.071	19.504	1.00	87.67	A
	593	OH	TYR	598	45.103	-6.015	20.464	1.00	89.91	A
55	594	C	TYR	598	42.607	-0.302	15.767	1.00	78.74	A
	595	O	TYR	598	42.158	0.582	16.490	1.00	79.40	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	596	N	SER	599	42.949	-0.111	14.502	1.00	77.13	A
	597	CA	SER	599	42.945	1.215	13.915	1.00	75.64	A
10	598	CB	SER	599	44.271	1.425	13.187	1.00	76.43	A
	599	OG	SER	599	44.381	0.534	12.088	1.00	77.42	A
	600	C	SER	599	41.816	1.623	12.978	1.00	73.69	A
	601	O	SER	599	41.908	2.674	12.347	1.00	73.01	A
15	602	N	TRP	600	40.752	0.840	12.882	1.00	72.01	A
	603	CA	TRP	600	39.696	1.228	11.962	1.00	70.02	A
	604	CB	TRP	600	38.635	0.102	11.860	1.00	68.48	A
20	605	CG	TRP	600	37.721	-0.054	13.036	1.00	67.90	A
	606	CD2	TRP	600	36.434	0.550	13.179	1.00	67.96	A
	607	CE2	TRP	600	35.960	0.229	14.472	1.00	67.86	A
	608	CE3	TRP	600	35.616	1.302	12.326	1.00	66.28	A
25	609	CD1	TRP	600	37.984	-0.689	14.220	1.00	67.57	A
	610	NE1	TRP	600	36.932	-0.516	15.094	1.00	67.79	A
	611	CZ2	TRP	600	34.733	0.684	14.957	1.00	67.32	A
30	612	CZ3	TRP	600	34.400	1.751	12.797	1.00	67.02	A
	613	CH2	TRP	600	33.959	1.426	14.098	1.00	67.80	A
	614	C	TRP	600	39.062	2.615	12.252	1.00	69.26	A
	615	O	TRP	600	38.704	3.343	11.321	1.00	68.40	A
35	616	N	MET	601	38.954	3.014	13.516	1.00	68.05	A
	617	CA	MET	601	38.354	4.317	13.800	1.00	67.13	A
	618	CB	MET	601	37.794	4.349	15.218	1.00	68.03	A
40	619	CG	MET	601	36.990	5.601	15.536	1.00	68.98	A
	620	SD	MET	601	35.331	5.636	14.826	1.00	69.62	A
	621	CE	MET	601	34.434	4.799	16.078	1.00	69.04	A
	622	C	MET	601	39.378	5.439	13.613	1.00	66.32	A
45	623	O	MET	601	39.055	6.524	13.120	1.00	65.08	A
	624	N	SER	602	40.612	5.174	14.016	1.00	65.58	A
	625	CA	SER	602	41.668	6.157	13.858	1.00	64.76	A
50	626	CB	SER	602	43.018	5.519	14.185	1.00	65.19	A
	627	OG	SER	602	44.010	6.500	14.419	1.00	66.76	A
	628	C	SER	602	41.610	6.568	12.387	1.00	63.83	A
	629	O	SER	602	41.581	7.753	12.058	1.00	63.81	A
55	630	N	LEU	603	41.546	5.564	11.512	1.00	63.22	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	631	CA	LEU	603	41.485	5.746	10.059	1.00	61.75	A
	632	CB	LEU	603	41.555	4.393	9.364	1.00	60.69	A
10	633	CG	LEU	603	42.781	3.526	9.588	1.00	59.23	A
	634	CD1	LEU	603	42.470	2.124	9.100	1.00	59.85	A
	635	CD2	LEU	603	43.981	4.120	8.876	1.00	58.03	A
15	636	C	LEU	603	40.227	6.451	9.553	1.00	61.71	A
	637	O	LEU	603	40.308	7.366	8.740	1.00	60.08	A
	638	N	MET	604	39.071	5.974	10.005	1.00	62.13	A
	639	CA	MET	604	37.786	6.525	9.603	1.00	62.89	A
20	640	CB	MET	604	36.645	5.671	10.186	1.00	64.15	A
	641	CG	MET	604	35.998	4.681	9.194	1.00	64.86	A
	642	SD	MET	604	37.123	4.017	7.921	1.00	69.00	A
25	643	CE	MET	604	36.833	5.103	6.468	1.00	67.97	A
	644	C	MET	604	37.675	7.995	10.031	1.00	63.55	A
	645	O	MET	604	37.309	8.854	9.228	1.00	64.56	A
	646	N	ALA	605	38.025	8.294	11.283	1.00	63.18	A
30	647	CA	ALA	605	37.959	9.674	11.761	1.00	61.86	A
	648	CB	ALA	605	38.021	9.719	13.291	1.00	61.77	A
	649	C	ALA	605	39.052	10.556	11.155	1.00	61.28	A
35	650	O	ALA	605	38.801	11.720	10.857	1.00	63.43	A
	651	N	PHE	606	40.256	10.033	10.963	1.00	59.86	A
	652	CA	PHE	606	41.308	10.852	10.368	1.00	59.36	A
40	653	CB	PHE	606	42.662	10.124	10.405	1.00	57.40	A
	654	CG	PHE	606	43.820	10.993	10.011	1.00	55.08	A
	655	CD1	PHE	606	44.153	12.110	10.770	1.00	53.58	A
	656	CD2	PHE	606	44.515	10.755	8.837	1.00	54.57	A
45	657	CE1	PHE	606	45.162	12.979	10.367	1.00	53.02	A
	658	CE2	PHE	606	45.537	11.627	8.423	1.00	54.27	A
	659	CZ	PHE	606	45.852	12.741	9.187	1.00	52.34	A
	660	C	PHE	606	40.945	11.236	8.916	1.00	60.57	A
50	661	O	PHE	606	41.380	12.270	8.401	1.00	61.01	A
	662	N	ALA	607	40.140	10.412	8.257	1.00	61.24	A
	663	CA	ALA	607	39.734	10.706	6.890	1.00	60.99	A
55	664	CB	ALA	607	39.229	9.456	6.212	1.00	62.48	A
	665	C	ALA	607	38.654	11.786	6.870	1.00	60.76	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
666	O	ALA	607	38.758	12.748	6.107	1.00	60.48	A
667	N	LEU	608	37.611	11.629	7.687	1.00	59.85	A
668	CA	LEU	608	36.561	12.644	7.738	1.00	60.59	A
669	CB	LEU	608	35.499	12.267	8.773	1.00	60.18	A
670	CG	LEU	608	34.414	13.234	9.264	1.00	61.39	A
671	CD1	LEU	608	33.099	13.239	8.441	1.00	62.18	A
672	CD2	LEU	608	34.119	12.747	10.668	1.00	60.55	A
673	C	LEU	608	37.247	13.966	8.093	1.00	61.63	A
674	O	LEU	608	37.031	14.972	7.416	1.00	61.28	A
675	N	GLY	609	38.095	13.974	9.125	1.00	61.90	A
676	CA	GLY	609	38.785	15.206	9.448	1.00	62.07	A
677	C	GLY	609	39.165	15.873	8.130	1.00	62.66	A
678	O	GLY	609	38.727	16.974	7.810	1.00	63.76	A
679	N	TRP	610	39.955	15.162	7.336	1.00	62.36	A
680	CA	TRP	610	40.419	15.637	6.040	1.00	60.84	A
681	CB	TRP	610	41.207	14.528	5.364	1.00	57.02	A
682	CG	TRP	610	41.865	14.975	4.130	1.00	52.45	A
683	CD2	TRP	610	43.040	15.777	4.054	1.00	50.06	A
684	CE2	TRP	610	43.335	15.952	2.684	1.00	48.16	A
685	CE3	TRP	610	43.842	16.405	5.019	1.00	49.35	A
686	CD1	TRP	610	41.511	14.679	2.839	1.00	50.18	A
687	NE1	TRP	610	42.404	15.259	1.967	1.00	48.49	A
688	CZ2	TRP	610	44.446	16.684	2.250	1.00	49.59	A
689	CZ3	TRP	610	44.948	17.142	4.592	1.00	49.89	A
690	CH2	TRP	610	45.227	17.292	3.210	1.00	50.85	A
691	C	TRP	610	39.353	16.134	5.059	1.00	61.87	A
692	O	TRP	610	39.468	17.219	4.504	1.00	62.11	A
693	N	ARG	611	38.337	15.321	4.808	1.00	63.21	A
694	CA	ARG	611	37.300	15.718	3.873	1.00	64.73	A
695	CB	ARG	611	36.250	14.611	3.737	1.00	65.43	A
696	CG	ARG	611	36.749	13.336	3.066	1.00	64.87	A
697	CD	ARG	611	35.582	12.508	2.553	1.00	64.94	A
698	NE	ARG	611	34.683	12.093	3.628	1.00	66.13	A
699	CZ	ARG	611	35.034	11.266	4.605	1.00	66.82	A
700	NH1	ARG	611	36.270	10.765	4.637	1.00	67.98	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	701	NH2	ARG	611	34.147	10.908	5.532	1.00	64.34	A
	702	C	ARG	611	36.646	16.998	4.379	1.00	66.30	A
10	703	O	ARG	611	36.212	17.848	3.596	1.00	67.09	A
	704	N	SER	612	36.604	17.134	5.696	1.00	67.15	A
	705	CA	SER	612	36.007	18.294	6.336	1.00	67.98	A
15	706	CB	SER	612	35.798	18.004	7.807	1.00	66.31	A
	707	OG	SER	612	34.810	17.005	7.922	1.00	66.23	A
	708	C	SER	612	36.830	19.548	6.183	1.00	69.48	A
	709	O	SER	612	36.322	20.611	5.834	1.00	69.46	A
20	710	N	TYR	613	38.107	19.429	6.473	1.00	71.12	A
	711	CA	TYR	613	38.963	20.571	6.348	1.00	74.12	A
	712	CB	TYR	613	40.343	20.137	6.799	1.00	72.89	A
25	713	CG	TYR	613	41.520	20.770	6.137	1.00	72.72	A
	714	CD1	TYR	613	41.827	22.116	6.316	1.00	71.49	A
	715	CE1	TYR	613	43.039	22.638	5.861	1.00	71.14	A
	716	CD2	TYR	613	42.437	19.967	5.467	1.00	73.13	A
30	717	CE2	TYR	613	43.636	20.472	5.009	1.00	73.12	A
	718	CZ	TYR	613	43.941	21.799	5.214	1.00	71.86	A
	719	OH	TYR	613	45.173	22.250	4.807	1.00	71.29	A
35	720	C	TYR	613	38.914	21.029	4.893	1.00	76.62	A
	721	O	TYR	613	38.594	22.176	4.598	1.00	77.91	A
	722	N	ARG	614	39.149	20.108	3.982	1.00	79.53	A
	723	CA	ARG	614	39.169	20.433	2.563	1.00	82.42	A
40	724	CB	ARG	614	39.712	19.213	1.827	1.00	83.40	A
	725	CG	ARG	614	41.000	18.718	2.460	1.00	84.51	A
	726	CD	ARG	614	42.108	19.638	2.084	1.00	84.98	A
45	727	NE	ARG	614	42.150	19.612	0.637	1.00	87.19	A
	728	CZ	ARG	614	43.238	19.787	-0.094	1.00	89.15	A
	729	NH1	ARG	614	44.414	20.020	0.490	1.00	89.01	A
	730	NH2	ARG	614	43.150	19.678	-1.414	1.00	89.92	A
50	731	C	ARG	614	37.866	20.913	1.904	1.00	83.98	A
	732	O	ARG	614	37.896	21.448	0.794	1.00	83.82	A
	733	N	GLN	615	36.731	20.766	2.586	1.00	85.72	A
55	734	CA	GLN	615	35.446	21.126	1.990	1.00	87.80	A
	735	CB	GLN	615	34.641	19.833	1.811	1.00	88.02	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
736	CG	GLN	615	33.302	19.930	1.105	1.00	89.29	A
737	CD	GLN	615	32.464	18.668	1.302	1.00	90.00	A
738	OE1	GLN	615	31.230	18.697	1.191	1.00	89.30	A
739	NE2	GLN	615	33.131	17.549	1.598	1.00	90.17	A
740	C	GLN	615	34.621	22.153	2.763	1.00	89.16	A
741	O	GLN	615	33.419	22.280	2.541	1.00	89.38	A
742	N	SER	616	35.259	22.894	3.663	1.00	90.80	A
743	CA	SER	616	34.543	23.885	4.457	1.00	92.99	A
744	CB	SER	616	33.235	23.296	5.016	1.00	92.42	A
745	OG	SER	616	33.445	22.457	6.143	1.00	90.39	A
746	C	SER	616	35.431	24.338	5.603	1.00	95.02	A
747	O	SER	616	34.953	24.572	6.711	1.00	95.57	A
748	N	SER	617	36.723	24.445	5.333	1.00	96.67	A
749	CA	SER	617	37.700	24.867	6.337	1.00	98.08	A
750	CB	SER	617	37.677	26.400	6.509	1.00	98.21	A
751	OG	SER	617	37.701	27.099	5.276	1.00	98.06	A
752	C	SER	617	37.510	24.244	7.730	1.00	98.69	A
753	O	SER	617	37.895	24.856	8.724	1.00	99.28	A
754	N	ALA	618	36.912	23.060	7.831	1.00	98.75	A
755	CA	ALA	618	36.743	22.448	9.156	1.00	99.29	A
756	CB	ALA	618	38.080	22.494	9.915	1.00	98.81	A
757	C	ALA	618	35.631	23.069	10.026	1.00	99.45	A
758	O	ALA	618	35.706	23.014	11.264	1.00	99.79	A
759	N	ASN	619	34.616	23.645	9.378	1.00	98.51	A
760	CA	ASN	619	33.466	24.275	10.044	1.00	97.30	A
761	CB	ASN	619	32.907	25.407	9.168	1.00	97.72	A
762	CG	ASN	619	33.993	26.254	8.533	1.00	97.81	A
763	OD1	ASN	619	33.766	26.909	7.510	1.00	97.90	A
764	ND2	ASN	619	35.175	26.254	9.137	1.00	97.55	A
765	C	ASN	619	32.370	23.216	10.191	1.00	96.23	A
766	O	ASN	619	31.673	23.120	11.208	1.00	95.29	A
767	N	LEU	620	32.238	22.430	9.127	1.00	94.73	A
768	CA	LEU	620	31.260	21.363	9.020	1.00	92.84	A
769	CB	LEU	620	30.476	21.547	7.705	1.00	92.98	A
770	CG	LEU	620	29.802	22.919	7.492	1.00	92.80	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	771	CD1	LEU	620	28.936	22.943	6.226	1.00	92.07	A
	772	CD2	LEU	620	28.939	23.220	8.704	1.00	92.73	A
10	773	C	LEU	620	31.983	19.998	9.044	1.00	91.47	A
	774	O	LEU	620	33.207	19.941	8.910	1.00	91.02	A
	775	N	LEU	621	31.229	18.918	9.256	1.00	89.67	A
15	776	CA	LEU	621	31.757	17.547	9.256	1.00	87.87	A
	777	CB	LEU	621	31.206	16.722	10.430	1.00	87.01	A
	778	CG	LEU	621	31.886	16.853	11.791	1.00	86.70	A
	779	CD1	LEU	621	31.304	15.830	12.766	1.00	86.15	A
20	780	CD2	LEU	621	33.378	16.639	11.623	1.00	85.78	A
	781	C	LEU	621	31.230	16.961	7.962	1.00	86.90	A
	782	O	LEU	621	30.029	16.809	7.805	1.00	86.82	A
25	783	N	CYS	622	32.112	16.619	7.032	1.00	85.92	A
	784	CA	CYS	622	31.639	16.104	5.753	1.00	85.59	A
	785	CB	CYS	622	32.449	16.744	4.629	1.00	85.97	A
	786	SG	CYS	622	32.515	18.552	4.739	1.00	88.73	A
30	787	C	CYS	622	31.669	14.596	5.612	1.00	84.70	A
	788	O	CYS	622	32.503	14.057	4.892	1.00	85.08	A
	789	N	PHE	623	30.751	13.902	6.264	1.00	83.91	A
35	790	CA	PHE	623	30.761	12.459	6.154	1.00	83.55	A
	791	CB	PHE	623	29.637	11.864	7.015	1.00	81.77	A
	792	CG	PHE	623	29.897	11.980	8.515	1.00	80.87	A
	793	CD1	PHE	623	29.644	13.162	9.210	1.00	80.74	A
40	794	CD2	PHE	623	30.380	10.890	9.235	1.00	80.88	A
	795	CE1	PHE	623	29.870	13.256	10.601	1.00	80.30	A
	796	CE2	PHE	623	30.612	10.979	10.615	1.00	80.14	A
45	797	CZ	PHE	623	30.350	12.159	11.297	1.00	80.61	A
	798	C	PHE	623	30.754	11.990	4.674	1.00	84.77	A
	799	O	PHE	623	31.382	10.986	4.343	1.00	85.60	A
50	800	N	ALA	624	30.089	12.730	3.790	1.00	85.86	A
	801	CA	ALA	624	30.081	12.431	2.348	1.00	87.32	A
	802	CB	ALA	624	28.888	11.576	1.985	1.00	86.51	A
	803	C	ALA	624	29.974	13.821	1.713	1.00	88.99	A
55	804	O	ALA	624	29.353	14.699	2.307	1.00	89.36	A
	805	N	PRO	625	30.590	14.071	0.532	1.00	90.51	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
806	CD	PRO	625	31.601	13.375	-0.288	1.00	91.20	A
807	CA	PRO	625	30.404	15.451	0.055	1.00	91.39	A
808	CB	PRO	625	31.248	15.492	-1.223	1.00	91.01	A
809	CG	PRO	625	32.366	14.540	-0.909	1.00	90.40	A
810	C	PRO	625	28.929	15.814	-0.180	1.00	91.81	A
811	O	PRO	625	28.590	16.979	-0.420	1.00	91.56	A
812	N	ASP	626	28.071	14.797	-0.077	1.00	91.89	A
813	CA	ASP	626	26.623	14.915	-0.260	1.00	91.87	A
814	CB	ASP	626	26.103	13.750	-1.069	1.00	93.67	A
815	CG	ASP	626	26.079	12.476	-0.245	1.00	95.47	A
816	OD1	ASP	626	27.157	12.118	0.255	1.00	97.06	A
817	OD2	ASP	626	25.008	11.853	-0.069	1.00	95.89	A
818	C	ASP	626	25.877	14.820	1.071	1.00	91.25	A
819	O	ASP	626	24.658	14.974	1.104	1.00	92.29	A
820	N	LEU	627	26.581	14.500	2.148	1.00	90.06	A
821	CA	LEU	627	25.926	14.362	3.447	1.00	88.48	A
822	CB	LEU	627	25.801	12.876	3.806	1.00	86.93	A
823	CG	LEU	627	25.003	12.516	5.059	1.00	86.55	A
824	CD1	LEU	627	25.598	13.155	6.301	1.00	86.49	A
825	CD2	LEU	627	23.588	12.986	4.868	1.00	86.46	A
826	C	LEU	627	26.721	15.104	4.520	1.00	87.74	A
827	O	LEU	627	27.639	14.539	5.114	1.00	88.20	A
828	N	ILE	628	26.352	16.356	4.776	1.00	86.51	A
829	CA	ILE	628	27.046	17.208	5.752	1.00	84.81	A
830	CB	ILE	628	27.296	18.638	5.173	1.00	83.92	A
831	CG2	ILE	628	27.963	19.516	6.212	1.00	83.50	A
832	CG1	ILE	628	28.228	18.585	3.964	1.00	83.63	A
833	CD1	ILE	628	27.752	17.707	2.855	1.00	83.66	A
834	C	ILE	628	26.327	17.405	7.091	1.00	84.24	A
835	O	ILE	628	25.099	17.397	7.167	1.00	84.45	A
836	N	ILE	629	27.097	17.566	8.161	1.00	83.48	A
837	CA	ILE	629	26.461	17.844	9.428	1.00	82.78	A
838	CB	ILE	629	26.999	17.048	10.607	1.00	81.63	A
839	CG2	ILE	629	26.599	17.734	11.903	1.00	79.75	A
840	CG1	ILE	629	26.470	15.604	10.547	1.00	82.25	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	841	CD1	ILE	629	25.110	15.415	9.861	1.00	81.23	A
	842	C	ILE	629	26.697	19.304	9.659	1.00	83.83	A
10	843	O	ILE	629	27.797	19.755	9.985	1.00	83.14	A
	844	N	ASN	630	25.607	20.021	9.437	1.00	85.68	A
	845	CA	ASN	630	25.502	21.453	9.547	1.00	86.72	A
15	846	CB	ASN	630	24.607	21.962	8.456	1.00	86.20	A
	847	CG	ASN	630	23.272	21.261	8.477	1.00	85.18	A
	848	OD1	ASN	630	22.946	20.552	9.426	1.00	84.86	A
	849	ND2	ASN	630	22.492	21.447	7.437	1.00	84.97	A
20	850	C	ASN	630	24.868	21.858	10.857	1.00	88.22	A
	851	O	ASN	630	24.323	21.039	11.613	1.00	87.63	A
	852	N	GLU	631	24.872	23.179	11.018	1.00	90.31	A
25	853	CA	GLU	631	24.398	23.891	12.187	1.00	91.48	A
	854	CB	GLU	631	24.382	25.385	11.921	1.00	93.00	A
	855	CG	GLU	631	23.793	26.104	13.115	1.00	96.45	A
	856	CD	GLU	631	23.464	27.561	12.874	1.00	98.56	A
30	857	OE1	GLU	631	22.255	27.889	12.773	1.00	98.65	A
	858	OE2	GLU	631	24.414	28.374	12.797	1.00	99.30	A
	859	C	GLU	631	23.060	23.541	12.736	1.00	91.50	A
35	860	O	GLU	631	22.827	23.560	13.943	1.00	91.38	A
	861	N	GLN	632	22.164	23.270	11.820	1.00	91.77	A
	862	CA	GLN	632	20.832	22.950	12.183	1.00	92.07	A
	863	CB	GLN	632	19.965	23.198	10.992	1.00	93.94	A
40	864	CG	GLN	632	19.286	24.573	10.860	1.00	97.21	A
	865	CD	GLN	632	19.518	25.646	11.945	1.00	98.67	A
	866	OE1	GLN	632	19.142	25.505	13.107	1.00	99.98	A
45	867	NE2	GLN	632	20.095	26.764	11.526	1.00	99.13	A
	868	C	GLN	632	20.837	21.487	12.542	1.00	90.67	A
	869	O	GLN	632	20.097	21.044	13.410	1.00	91.24	A
	870	N	ARG	633	21.686	20.733	11.873	1.00	89.18	A
50	871	CA	ARG	633	21.775	19.313	12.161	1.00	87.17	A
	872	CB	ARG	633	22.453	18.598	11.021	1.00	86.70	A
	873	CG	ARG	633	21.431	17.895	10.184	1.00	84.53	A
55	874	CD	ARG	633	22.020	17.447	8.896	1.00	83.94	A
	875	NE	ARG	633	21.077	16.992	7.877	1.00	82.31	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
876	CZ	ARG	633	21.490	16.771	6.637	1.00	80.78	A
877	NH1	ARG	633	22.767	16.982	6.379	1.00	81.48	A
878	NH2	ARG	633	20.673	16.342	5.682	1.00	78.84	A
879	C	ARG	633	22.586	19.091	13.403	1.00	86.42	A
880	O	ARG	633	22.417	18.149	14.163	1.00	86.50	A
881	N	MET	634	23.508	19.990	13.583	1.00	85.41	A
882	CA	MET	634	24.422	19.923	14.676	1.00	85.16	A
883	CB	MET	634	25.333	21.071	14.564	1.00	83.80	A
884	CG	MET	634	26.532	20.722	15.242	1.00	83.67	A
885	SD	MET	634	26.813	18.971	14.989	1.00	83.03	A
886	CE	MET	634	28.456	18.959	15.223	1.00	81.55	A
887	C	MET	634	23.750	20.066	15.958	1.00	85.63	A
888	O	MET	634	24.225	19.776	17.058	1.00	85.09	A
889	N	THR	635	22.601	20.597	15.781	1.00	87.23	A
890	CA	THR	635	21.881	20.899	16.896	1.00	88.52	A
891	CB	THR	635	21.350	22.196	16.587	1.00	87.94	A
892	OG1	THR	635	20.215	22.470	17.380	1.00	89.21	A
893	CG2	THR	635	20.985	22.182	15.195	1.00	88.12	A
894	C	THR	635	20.853	19.841	17.202	1.00	89.56	A
895	O	THR	635	19.970	20.116	17.985	1.00	90.59	A
896	N	LEU	636	20.892	18.633	16.625	1.00	89.94	A
897	CA	LEU	636	19.861	17.719	17.107	1.00	90.42	A
898	CB	LEU	636	19.555	16.490	16.236	1.00	91.24	A
899	CG	LEU	636	19.136	16.816	14.826	1.00	92.26	A
900	CD1	LEU	636	20.324	17.384	14.235	1.00	92.82	A
901	CD2	LEU	636	18.739	15.622	14.013	1.00	92.86	A
902	C	LEU	636	20.401	17.252	18.416	1.00	90.58	A
903	O	LEU	636	21.542	17.553	18.802	1.00	90.48	A
904	N	PRO	637	19.594	16.478	19.111	1.00	90.59	A
905	CD	PRO	637	18.305	15.875	18.738	1.00	90.32	A
906	CA	PRO	637	20.019	15.991	20.398	1.00	91.07	A
907	CB	PRO	637	19.091	14.825	20.639	1.00	90.73	A
908	CG	PRO	637	17.847	15.305	20.031	1.00	90.37	A
909	C	PRO	637	21.425	15.600	20.619	1.00	91.70	A
910	O	PRO	637	22.349	16.393	20.827	1.00	93.14	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	911	N	CYS	638	21.589	14.316	20.539	1.00	91.74	A
	912	CA	CYS	638	22.857	13.860	20.917	1.00	91.86	A
10	913	CB	CYS	638	22.672	12.435	21.382	1.00	91.44	A
	914	SG	CYS	638	22.362	12.383	23.136	1.00	92.33	A
	915	C	CYS	638	24.004	14.008	19.970	1.00	91.43	A
15	916	O	CYS	638	24.977	13.305	20.113	1.00	92.21	A
	917	N	MET	639	23.955	14.977	19.074	1.00	90.28	A
	918	CA	MET	639	25.003	15.076	18.076	1.00	89.06	A
	919	CB	MET	639	24.474	15.815	16.875	1.00	89.67	A
20	920	CG	MET	639	25.057	15.363	15.576	1.00	89.96	A
	921	SD	MET	639	23.803	14.471	14.669	1.00	91.78	A
	922	CE	MET	639	24.470	12.873	14.665	1.00	91.55	A
25	923	C	MET	639	26.280	15.742	18.432	1.00	88.30	A
	924	O	MET	639	27.390	15.236	18.249	1.00	88.54	A
	925	N	TYR	640	26.089	16.955	18.882	1.00	87.19	A
	926	CA	TYR	640	27.202	17.757	19.177	1.00	85.96	A
30	927	CB	TYR	640	26.724	19.072	19.707	1.00	83.25	A
	928	CG	TYR	640	27.903	19.924	19.724	1.00	81.17	A
	929	CD1	TYR	640	28.386	20.449	18.536	1.00	80.77	A
35	930	CE1	TYR	640	29.621	21.033	18.475	1.00	79.85	A
	931	CD2	TYR	640	28.685	20.016	20.866	1.00	79.86	A
	932	CE2	TYR	640	29.923	20.591	20.822	1.00	79.30	A
	933	CZ	TYR	640	30.388	21.095	19.622	1.00	79.94	A
40	934	OH	TYR	640	31.638	21.656	19.564	1.00	79.45	A
	935	C	TYR	640	28.230	17.187	20.119	1.00	86.91	A
	936	O	TYR	640	29.423	17.431	19.984	1.00	87.67	A
45	937	N	ASP	641	27.773	16.429	21.093	1.00	88.23	A
	938	CA	ASP	641	28.693	15.872	22.061	1.00	89.33	A
	939	CB	ASP	641	27.933	15.217	23.184	1.00	91.25	A
	940	CG	ASP	641	27.827	16.076	24.402	1.00	92.97	A
50	941	OD1	ASP	641	28.852	16.625	24.886	1.00	93.24	A
	942	OD2	ASP	641	26.684	16.169	24.889	1.00	93.94	A
	943	C	ASP	641	29.574	14.812	21.474	1.00	89.35	A
55	944	O	ASP	641	30.653	14.546	21.979	1.00	89.26	A
	945	N	GLN	642	29.045	14.178	20.434	1.00	89.50	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
946	CA	GLN	642	29.666	13.099	19.688	1.00	89.13	A
947	CB	GLN	642	28.526	12.237	19.044	1.00	90.27	A
948	CG	GLN	642	27.962	10.822	19.594	1.00	91.79	A
949	CD	GLN	642	26.681	10.417	18.792	1.00	93.88	A
950	OE1	GLN	642	26.221	9.266	18.765	1.00	94.69	A
951	NE2	GLN	642	26.098	11.421	18.152	1.00	94.27	A
952	C	GLN	642	30.568	13.716	18.613	1.00	88.31	A
953	O	GLN	642	31.765	13.430	18.522	1.00	87.84	A
954	N	CYS	643	29.961	14.599	17.822	1.00	87.09	A
955	CA	CYS	643	30.607	15.296	16.691	1.00	86.13	A
956	CB	CYS	643	29.579	16.175	15.965	1.00	85.59	A
957	SG	CYS	643	28.434	15.246	14.937	1.00	86.84	A
958	C	CYS	643	31.835	16.167	16.978	1.00	85.11	A
959	O	CYS	643	32.634	16.451	16.086	1.00	85.48	A
960	N	LYS	644	31.978	16.570	18.224	1.00	83.90	A
961	CA	LYS	644	33.050	17.445	18.689	1.00	82.99	A
962	CB	LYS	644	32.847	17.650	20.164	1.00	83.94	A
963	CG	LYS	644	33.903	18.465	20.828	1.00	84.87	A
964	CD	LYS	644	33.751	18.350	22.330	1.00	85.64	A
965	CE	LYS	644	32.292	18.434	22.762	1.00	86.34	A
966	NZ	LYS	644	32.193	18.431	24.245	1.00	85.91	A
967	C	LYS	644	34.451	16.938	18.505	1.00	82.08	A
968	O	LYS	644	35.424	17.654	18.224	1.00	81.31	A
969	N	HIS	645	34.526	15.664	18.775	1.00	81.67	A
970	CA	HIS	645	35.747	14.987	18.710	1.00	81.48	A
971	CB	HIS	645	35.510	13.663	19.317	1.00	83.43	A
972	CG	HIS	645	35.703	13.776	20.783	1.00	85.32	A
973	CD2	HIS	645	36.806	14.279	21.392	1.00	86.28	A
974	ND1	HIS	645	34.689	13.785	21.664	1.00	86.22	A
975	CE1	HIS	645	35.135	14.319	22.824	1.00	87.26	A
976	NE2	HIS	645	36.392	14.616	22.663	1.00	87.68	A
977	C	HIS	645	36.286	14.967	17.372	1.00	80.40	A
978	O	HIS	645	37.442	15.286	17.131	1.00	79.49	A
979	N	MET	646	35.403	14.670	16.460	1.00	79.68	A
980	CA	MET	646	35.847	14.655	15.125	1.00	78.11	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	981	CB	MET	646	34.794	14.004	14.287	1.00	78.69	A
	982	CG	MET	646	34.894	12.531	14.452	1.00	78.50	A
10	983	SD	MET	646	33.445	11.861	15.209	1.00	80.06	A
	984	CE	MET	646	32.393	11.981	13.892	1.00	82.37	A
	985	C	MET	646	36.199	16.020	14.595	1.00	76.66	A
15	986	O	MET	646	37.186	16.151	13.878	1.00	76.52	A
	987	N	LEU	647	35.414	17.042	14.944	1.00	75.12	A
	988	CA	LEU	647	35.692	18.380	14.416	1.00	74.23	A
	989	CB	LEU	647	34.616	19.401	14.824	1.00	73.81	A
20	990	CG	LEU	647	33.384	19.749	13.952	1.00	72.95	A
	991	CD1	LEU	647	32.473	20.475	14.890	1.00	73.14	A
	992	CD2	LEU	647	33.651	20.650	12.712	1.00	74.46	A
25	993	C	LEU	647	37.038	18.786	14.921	1.00	73.06	A
	994	O	LEU	647	37.798	19.493	14.267	1.00	73.18	A
	995	N	TYR	648	37.343	18.325	16.105	1.00	71.81	A
	996	CA	TYR	648	38.626	18.614	16.615	1.00	70.55	A
30	997	CB	TYR	648	38.770	17.967	17.942	1.00	71.32	A
	998	CG	TYR	648	40.193	17.938	18.201	1.00	72.59	A
	999	CD1	TYR	648	40.922	16.773	18.043	1.00	72.98	A
35	1000	CE1	TYR	648	42.276	16.793	18.159	1.00	74.89	A
	1001	CD2	TYR	648	40.849	19.122	18.479	1.00	73.43	A
	1002	CE2	TYR	648	42.193	19.160	18.595	1.00	74.28	A
	1003	CZ	TYR	648	42.909	17.992	18.446	1.00	75.87	A
40	1004	OH	TYR	648	44.259	18.004	18.666	1.00	78.05	A
	1005	C	TYR	648	39.727	18.082	15.672	1.00	69.47	A
	1006	O	TYR	648	40.782	18.697	15.527	1.00	69.10	A
45	1007	N	VAL	649	39.535	16.936	15.042	1.00	68.99	A
	1008	CA	VAL	649	40.641	16.531	14.205	1.00	68.88	A
	1009	CB	VAL	649	40.677	14.969	13.955	1.00	69.22	A
	1010	CG1	VAL	649	39.292	14.369	13.993	1.00	68.78	A
50	1011	CG2	VAL	649	41.391	14.663	12.652	1.00	69.29	A
	1012	C	VAL	649	40.674	17.386	12.935	1.00	68.29	A
	1013	O	VAL	649	41.747	17.830	12.515	1.00	67.00	A
55	1014	N	SER	650	39.507	17.680	12.368	1.00	69.10	A
	1015	CA	SER	650	39.425	18.528	11.170	1.00	69.39	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1016	CB	SER	650	37.979	18.727	10.752	1.00	69.29	A
1017	OG	SER	650	37.915	19.900	9.974	1.00	71.17	A
1018	C	SER	650	40.015	19.922	11.379	1.00	69.02	A
1019	O	SER	650	40.648	20.502	10.486	1.00	68.81	A
1020	N	SER	651	39.758	20.475	12.557	1.00	68.62	A
1021	CA	SER	651	40.248	21.799	12.916	1.00	68.72	A
1022	CB	SER	651	39.724	22.166	14.315	1.00	70.09	A
1023	OG	SER	651	40.748	22.677	15.162	1.00	72.58	A
1024	C	SER	651	41.772	21.790	12.913	1.00	67.36	A
1025	O	SER	651	42.430	22.683	12.379	1.00	66.28	A
1026	N	GLU	652	42.310	20.739	13.514	1.00	66.84	A
1027	CA	GLU	652	43.737	20.543	13.652	1.00	65.75	A
1028	CB	GLU	652	43.950	19.303	14.497	1.00	65.94	A
1029	CG	GLU	652	45.026	19.432	15.539	1.00	68.92	A
1030	CD	GLU	652	45.053	20.768	16.255	1.00	70.91	A
1031	OE1	GLU	652	44.020	21.469	16.341	1.00	72.27	A
1032	OE2	GLU	652	46.141	21.107	16.753	1.00	73.20	A
1033	C	GLU	652	44.472	20.448	12.323	1.00	64.24	A
1034	O	GLU	652	45.601	20.931	12.202	1.00	64.18	A
1035	N	LEU	653	43.838	19.818	11.339	1.00	63.37	A
1036	CA	LEU	653	44.407	19.689	9.997	1.00	62.68	A
1037	CB	LEU	653	43.515	18.797	9.117	1.00	60.31	A
1038	CG	LEU	653	43.496	17.298	9.453	1.00	58.08	A
1039	CD1	LEU	653	42.502	16.529	8.584	1.00	56.65	A
1040	CD2	LEU	653	44.889	16.766	9.259	1.00	55.94	A
1041	C	LEU	653	44.437	21.100	9.425	1.00	63.49	A
1042	O	LEU	653	45.454	21.574	8.919	1.00	63.20	A
1043	N	HIS	654	43.303	21.773	9.532	1.00	65.44	A
1044	CA	HIS	654	43.155	23.131	9.050	1.00	66.40	A
1045	CB	HIS	654	41.757	23.639	9.408	1.00	68.67	A
1046	CG	HIS	654	41.466	24.995	8.860	1.00	70.94	A
1047	CD2	HIS	654	40.952	25.380	7.669	1.00	72.19	A
1048	ND1	HIS	654	41.829	26.151	9.517	1.00	72.01	A
1049	CE1	HIS	654	41.561	27.190	8.743	1.00	72.60	A
1050	NE2	HIS	654	41.031	26.749	7.620	1.00	73.26	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1051	C	HIS	654	44.217	24.058	9.639	1.00	66.64	A
	1052	O	HIS	654	44.982	24.702	8.912	1.00	66.69	A
10	1053	N	ARG	655	44.253	24.114	10.964	1.00	66.13	A
	1054	CA	ARG	655	45.198	24.945	11.685	1.00	65.54	A
	1055	CB	ARG	655	45.095	24.674	13.168	1.00	66.61	A
15	1056	CG	ARG	655	45.840	25.672	14.004	1.00	68.07	A
	1057	CD	ARG	655	46.173	25.076	15.332	1.00	68.45	A
	1058	NE	ARG	655	47.501	24.497	15.290	1.00	71.04	A
	1059	CZ	ARG	655	47.952	23.630	16.183	1.00	73.26	A
20	1060	NH1	ARG	655	47.162	23.252	17.177	1.00	74.95	A
	1061	NH2	ARG	655	49.193	23.158	16.096	1.00	73.03	A
	1062	C	ARG	655	46.624	24.670	11.277	1.00	65.54	A
25	1063	O	ARG	655	47.460	25.575	11.222	1.00	66.10	A
	1064	N	LEU	656	46.920	23.408	11.014	1.00	65.42	A
	1065	CA	LEU	656	48.272	23.039	10.645	1.00	65.44	A
	1066	CB	LEU	656	48.584	21.653	11.206	1.00	64.44	A
30	1067	CG	LEU	656	49.148	21.728	12.619	1.00	63.25	A
	1068	CD1	LEU	656	49.549	20.337	13.064	1.00	63.29	A
	1069	CD2	LEU	656	50.358	22.650	12.625	1.00	62.26	A
35	1070	C	LEU	656	48.571	23.094	9.150	1.00	65.58	A
	1071	O	LEU	656	49.705	22.815	8.734	1.00	64.71	A
	1072	N	GLN	657	47.558	23.501	8.375	1.00	66.26	A
	1073	CA	GLN	657	47.599	23.588	6.907	1.00	67.33	A
40	1074	CB	GLN	657	48.272	24.883	6.412	1.00	70.37	A
	1075	CG	GLN	657	47.332	26.121	6.337	1.00	74.91	A
	1076	CD	GLN	657	46.109	25.932	5.418	1.00	77.90	A
45	1077	OE1	GLN	657	44.957	26.078	5.853	1.00	79.08	A
	1078	NE2	GLN	657	46.362	25.622	4.145	1.00	79.44	A
	1079	C	GLN	657	48.306	22.374	6.365	1.00	66.01	A
	1080	O	GLN	657	49.342	22.467	5.708	1.00	67.61	A
50	1081	N	VAL	658	47.714	21.224	6.663	1.00	64.56	A
	1082	CA	VAL	658	48.246	19.938	6.260	1.00	63.29	A
	1083	CB	VAL	658	47.627	18.787	7.098	1.00	61.27	A
55	1084	CG1	VAL	658	48.073	17.451	6.544	1.00	60.69	A
	1085	CG2	VAL	658	48.063	18.902	8.562	1.00	59.00	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1086	C	VAL	658	48.093	19.630	4.779	1.00	63.70	A
	1087	O	VAL	658	47.011	19.686	4.196	1.00	64.37	A
10	1088	N	SER	659	49.249	19.304	4.214	1.00	64.31	A
	1089	CA	SER	659	49.510	18.938	2.829	1.00	64.00	A
	1090	CB	SER	659	51.038	18.836	2.715	1.00	65.00	A
15	1091	OG	SER	659	51.521	18.491	1.435	1.00	68.63	A
	1092	C	SER	659	48.833	17.594	2.491	1.00	63.59	A
	1093	O	SER	659	48.599	16.781	3.384	1.00	63.80	A
	1094	N	TYR	660	48.512	17.353	1.219	1.00	62.62	A
20	1095	CA	TYR	660	47.894	16.080	0.862	1.00	60.90	A
	1096	CB	TYR	660	47.483	16.023	-0.603	1.00	57.88	A
	1097	CG	TYR	660	46.622	14.816	-0.889	1.00	55.47	A
25	1098	CD1	TYR	660	45.585	14.484	-0.024	1.00	54.48	A
	1099	CE1	TYR	660	44.729	13.439	-0.283	1.00	52.21	A
	1100	CD2	TYR	660	46.791	14.045	-2.044	1.00	53.60	A
	1101	CE2	TYR	660	45.926	12.977	-2.318	1.00	52.33	A
30	1102	CZ	TYR	660	44.892	12.692	-1.427	1.00	52.28	A
	1103	OH	TYR	660	43.969	11.695	-1.661	1.00	53.74	A
	1104	C	TYR	660	48.888	14.964	1.086	1.00	61.71	A
35	1105	O	TYR	660	48.546	13.894	1.581	1.00	62.27	A
	1106	N	GLU	661	50.129	15.213	0.693	1.00	62.99	A
	1107	CA	GLU	661	51.145	14.205	0.853	1.00	64.16	A
	1108	CB	GLU	661	52.430	14.641	0.165	1.00	65.20	A
40	1109	CG	GLU	661	52.264	14.520	-1.334	1.00	68.41	A
	1110	CD	GLU	661	53.567	14.573	-2.093	1.00	70.81	A
	1111	OE1	GLU	661	54.627	14.807	-1.463	1.00	69.79	A
45	1112	OE2	GLU	661	53.525	14.381	-3.331	1.00	73.10	A
	1113	C	GLU	661	51.338	13.912	2.319	1.00	63.87	A
	1114	O	GLU	661	51.208	12.760	2.734	1.00	64.43	A
	1115	N	GLU	662	51.626	14.943	3.107	1.00	62.73	A
50	1116	CA	GLU	662	51.788	14.740	4.535	1.00	60.94	A
	1117	CB	GLU	662	51.820	16.072	5.260	1.00	62.39	A
	1118	CG	GLU	662	53.120	16.809	5.171	1.00	63.89	A
55	1119	CD	GLU	662	52.926	18.276	5.467	1.00	65.88	A
	1120	OE1	GLU	662	51.759	18.720	5.449	1.00	66.26	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1121	OE2	GLU	662	53.923	18.992	5.705	1.00	66.78	A
	1122	C	GLU	662	50.611	13.923	5.068	1.00	59.42	A
10	1123	O	GLU	662	50.791	13.031	5.897	1.00	59.90	A
	1124	N	TYR	663	49.408	14.232	4.587	1.00	57.33	A
	1125	CA	TYR	663	48.182	13.546	5.016	1.00	57.29	A
15	1126	CB	TYR	663	46.944	14.179	4.372	1.00	55.05	A
	1127	CG	TYR	663	45.719	13.267	4.361	1.00	52.55	A
	1128	CD1	TYR	663	44.988	13.044	5.526	1.00	52.08	A
	1129	CE1	TYR	663	43.829	12.242	5.521	1.00	51.10	A
20	1130	CD2	TYR	663	45.272	12.661	3.180	1.00	51.77	A
	1131	CE2	TYR	663	44.114	11.856	3.161	1.00	50.54	A
	1132	CZ	TYR	663	43.390	11.656	4.340	1.00	51.46	A
25	1133	OH	TYR	663	42.207	10.922	4.350	1.00	52.74	A
	1134	C	TYR	663	48.114	12.068	4.685	1.00	57.96	A
	1135	O	TYR	663	47.530	11.268	5.430	1.00	58.51	A
	1136	N	LEU	664	48.652	11.726	3.520	1.00	58.19	A
30	1137	CA	LEU	664	48.629	10.366	3.047	1.00	57.31	A
	1138	CB	LEU	664	49.030	10.342	1.576	1.00	56.51	A
	1139	CG	LEU	664	47.854	10.677	0.655	1.00	54.66	A
35	1140	CD1	LEU	664	48.206	10.343	-0.776	1.00	54.06	A
	1141	CD2	LEU	664	46.639	9.867	1.068	1.00	52.20	A
	1142	C	LEU	664	49.547	9.511	3.890	1.00	57.26	A
	1143	O	LEU	664	49.257	8.342	4.184	1.00	56.63	A
40	1144	N	CYS	665	50.652	10.128	4.290	1.00	56.70	A
	1145	CA	CYS	665	51.629	9.475	5.118	1.00	57.53	A
	1146	CB	CYS	665	52.910	10.292	5.130	1.00	58.19	A
45	1147	SG	CYS	665	53.830	10.095	3.584	1.00	63.72	A
	1148	C	CYS	665	51.099	9.299	6.527	1.00	57.62	A
	1149	O	CYS	665	51.156	8.203	7.082	1.00	59.12	A
	1150	N	MET	666	50.557	10.362	7.109	1.00	57.03	A
50	1151	CA	MET	666	50.042	10.272	8.468	1.00	56.19	A
	1152	CB	MET	666	49.433	11.608	8.895	1.00	55.82	A
	1153	CG	MET	666	50.475	12.699	9.005	1.00	57.38	A
55	1154	SD	MET	666	49.817	14.370	9.027	1.00	58.37	A
	1155	CE	MET	666	49.222	14.475	10.771	1.00	59.18	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1156	C	MET	666	49.012	9.180	8.638	1.00	55.71	A
1157	O	MET	666	48.930	8.555	9.693	1.00	56.57	A
1158	N	LYS	667	48.225	8.937	7.603	1.00	55.23	A
1159	CA	LYS	667	47.178	7.935	7.730	1.00	54.64	A
1160	CB	LYS	667	46.097	8.190	6.698	1.00	53.25	A
1161	CG	LYS	667	44.903	7.301	6.845	1.00	52.56	A
1162	CD	LYS	667	43.726	7.893	6.096	1.00	52.52	A
1163	CE	LYS	667	44.050	8.168	4.637	1.00	51.07	A
1164	NZ	LYS	667	44.186	6.900	3.877	1.00	54.84	A
1165	C	LYS	667	47.693	6.506	7.631	1.00	54.78	A
1166	O	LYS	667	47.056	5.577	8.127	1.00	55.27	A
1167	N	THR	668	48.838	6.332	6.983	1.00	55.22	A
1168	CA	THR	668	49.433	5.013	6.850	1.00	55.52	A
1169	CB	THR	668	50.550	5.021	5.773	1.00	54.91	A
1170	OG1	THR	668	50.007	5.511	4.538	1.00	55.09	A
1171	CG2	THR	668	51.083	3.620	5.535	1.00	54.29	A
1172	C	THR	668	49.996	4.765	8.243	1.00	54.90	A
1173	O	THR	668	49.851	3.674	8.793	1.00	54.89	A
1174	N	LEU	669	50.602	5.803	8.828	1.00	55.28	A
1175	CA	LEU	669	51.151	5.714	10.182	1.00	55.00	A
1176	CB	LEU	669	51.890	7.001	10.566	1.00	52.74	A
1177	CG	LEU	669	53.266	7.224	9.928	1.00	51.51	A
1178	CD1	LEU	669	53.925	8.432	10.516	1.00	51.09	A
1179	CD2	LEU	669	54.144	6.030	10.175	1.00	51.14	A
1180	C	LEU	669	50.049	5.444	11.214	1.00	55.52	A
1181	O	LEU	669	50.321	4.968	12.311	1.00	56.72	A
1182	N	LEU	670	48.805	5.734	10.875	1.00	55.19	A
1183	CA	LEU	670	47.737	5.504	11.832	1.00	55.37	A
1184	CB	LEU	670	46.566	6.432	11.512	1.00	54.24	A
1185	CG	LEU	670	46.048	7.483	12.498	1.00	53.91	A
1186	CD1	LEU	670	47.100	8.401	13.059	1.00	51.87	A
1187	CD2	LEU	670	45.063	8.287	11.712	1.00	56.32	A
1188	C	LEU	670	47.282	4.044	11.849	1.00	56.26	A
1189	O	LEU	670	46.659	3.590	12.806	1.00	56.76	A
1190	N	LEU	671	47.583	3.314	10.784	1.00	57.62	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1191	CA	LEU	671	47.216	1.910	10.685	1.00	58.03	A
	1192	CB	LEU	671	47.306	1.483	9.207	1.00	54.95	A
10	1193	CG	LEU	671	47.458	0.030	8.739	1.00	52.63	A
	1194	CD1	LEU	671	46.215	-0.742	9.077	1.00	51.93	A
	1195	CD2	LEU	671	47.696	-0.023	7.234	1.00	51.62	A
15	1196	C	LEU	671	48.233	1.167	11.559	1.00	61.12	A
	1197	O	LEU	671	47.900	0.228	12.291	1.00	62.38	A
	1198	N	LEU	672	49.470	1.653	11.511	1.00	63.00	A
	1199	CA	LEU	672	50.578	1.073	12.259	1.00	63.98	A
20	1200	CB	LEU	672	51.843	1.143	11.395	1.00	60.71	A
	1201	CG	LEU	672	51.592	0.994	9.888	1.00	58.47	A
	1202	CD1	LEU	672	52.875	1.217	9.095	1.00	56.96	A
25	1203	CD2	LEU	672	51.013	-0.383	9.621	1.00	56.80	A
	1204	C	LEU	672	50.826	1.802	13.586	1.00	66.42	A
	1205	O	LEU	672	51.977	1.885	14.027	1.00	67.06	A
	1206	N	SER	673	49.768	2.304	14.231	1.00	68.97	A
30	1207	CA	SER	673	49.936	3.061	15.476	1.00	72.55	A
	1208	CB	SER	673	49.203	4.398	15.391	1.00	71.35	A
	1209	OG	SER	673	47.818	4.198	15.201	1.00	70.80	A
35	1210	C	SER	673	49.584	2.383	16.798	1.00	75.85	A
	1211	O	SER	673	49.707	2.988	17.867	1.00	76.67	A
	1212	N	SER	674	49.095	1.152	16.737	1.00	79.23	A
	1213	CA	SER	674	48.844	0.423	17.968	1.00	82.13	A
40	1214	CB	SER	674	47.492	0.781	18.613	1.00	81.41	A
	1215	OG	SER	674	46.385	0.252	17.915	1.00	84.00	A
	1216	C	SER	674	48.970	-1.056	17.652	1.00	83.87	A
45	1217	O	SER	674	48.424	-1.556	16.661	1.00	84.21	A
	1218	N	VAL	675	49.776	-1.715	18.477	1.00	85.78	A
	1219	CA	VAL	675	50.056	-3.137	18.373	1.00	87.96	A
	1220	CB	VAL	675	51.556	-3.381	18.110	1.00	86.94	A
50	1221	CG1	VAL	675	51.926	-2.896	16.726	1.00	86.95	A
	1222	CG2	VAL	675	52.390	-2.658	19.159	1.00	87.12	A
	1223	C	VAL	675	49.668	-3.783	19.704	1.00	90.28	A
55	1224	O	VAL	675	49.483	-3.092	20.709	1.00	89.69	A
	1225	N	PRO	676	49.544	-5.124	19.726	1.00	93.03	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1226	CD	PRO	676	49.961	-6.005	18.630	1.00	93.57	A
1227	CA	PRO	676	49.182	-5.919	20.904	1.00	95.42	A
1228	CB	PRO	676	49.235	-7.354	20.380	1.00	94.95	A
1229	CG	PRO	676	49.127	-7.206	18.883	1.00	94.18	A
1230	C	PRO	676	50.243	-5.673	21.963	1.00	97.54	A
1231	O	PRO	676	51.352	-5.257	21.626	1.00	98.58	A
1232	N	LYS	677	49.933	-5.929	23.229	1.00	99.68	A
1233	CA	LYS	677	50.917	-5.693	24.286	1.00	101.53	A
1234	CB	LYS	677	50.295	-5.899	25.670	1.00	102.63	A
1235	CG	LYS	677	51.160	-5.381	26.824	1.00	103.79	A
1236	CD	LYS	677	51.244	-6.398	27.965	1.00	104.31	A
1237	CE	LYS	677	52.012	-7.633	27.522	1.00	104.35	A
1238	NZ	LYS	677	51.800	-8.827	28.387	1.00	105.00	A
1239	C	LYS	677	52.107	-6.628	24.116	1.00	102.18	A
1240	O	LYS	677	53.147	-6.458	24.761	1.00	101.68	A
1241	N	ASP	678	51.949	-7.615	23.240	1.00	102.84	A
1242	CA	ASP	678	53.009	-8.571	22.980	1.00	104.29	A
1243	CB	ASP	678	52.524	-9.988	23.281	1.00	106.29	A
1244	CG	ASP	678	51.908	-10.107	24.656	1.00	108.07	A
1245	OD1	ASP	678	52.320	-9.342	25.551	1.00	108.43	A
1246	OD2	ASP	678	51.025	-10.974	24.842	1.00	109.39	A
1247	C	ASP	678	53.469	-8.488	21.532	1.00	104.24	A
1248	O	ASP	678	53.859	-9.493	20.935	1.00	104.59	A
1249	N	GLY	679	53.424	-7.286	20.968	1.00	103.43	A
1250	CA	GLY	679	53.840	-7.135	19.590	1.00	101.95	A
1251	C	GLY	679	53.097	-8.131	18.724	1.00	101.17	A
1252	O	GLY	679	52.297	-8.936	19.203	1.00	100.48	A
1253	N	LEU	680	53.382	-8.097	17.432	1.00	100.20	A
1254	CA	LEU	680	52.707	-8.983	16.504	1.00	98.61	A
1255	CB	LEU	680	52.425	-8.208	15.229	1.00	98.06	A
1256	CG	LEU	680	52.093	-6.769	15.601	1.00	97.47	A
1257	CD1	LEU	680	52.560	-5.848	14.516	1.00	97.75	A
1258	CD2	LEU	680	50.615	-6.630	15.855	1.00	97.02	A
1259	C	LEU	680	53.547	-10.203	16.202	1.00	97.47	A
1260	O	LEU	680	54.561	-10.459	16.850	1.00	97.58	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1261	N	LYS	681	53.120	-10.968	15.211	1.00	96.17	A
	1262	CA	LYS	681	53.865	-12.143	14.837	1.00	95.16	A
10	1263	CB	LYS	681	52.937	-13.202	14.245	1.00	95.18	A
	1264	CG	LYS	681	51.846	-13.706	15.192	1.00	94.91	A
	1265	CD	LYS	681	51.184	-14.927	14.581	1.00	94.17	A
15	1266	CE	LYS	681	49.836	-15.278	15.191	1.00	93.86	A
	1267	NZ	LYS	681	49.185	-16.380	14.418	1.00	92.63	A
	1268	C	LYS	681	54.937	-11.770	13.828	1.00	95.02	A
	1269	O	LYS	681	55.736	-12.613	13.437	1.00	95.32	A
20	1270	N	SER	682	54.962	-10.511	13.397	1.00	95.00	A
	1271	CA	SER	682	55.981	-10.080	12.435	1.00	94.85	A
	1272	CB	SER	682	55.377	-9.946	11.029	1.00	94.61	A
25	1273	OG	SER	682	54.906	-11.193	10.549	1.00	92.86	A
	1274	C	SER	682	56.639	-8.761	12.842	1.00	94.58	A
	1275	O	SER	682	57.167	-8.028	12.004	1.00	94.56	A
	1276	N	GLN	683	56.616	-8.482	14.144	1.00	94.40	A
30	1277	CA	GLN	683	57.192	-7.269	14.710	1.00	94.48	A
	1278	CB	GLN	683	57.517	-7.477	16.180	1.00	95.06	A
	1279	CG	GLN	683	56.384	-7.111	17.096	1.00	97.14	A
35	1280	CD	GLN	683	56.186	-5.606	17.210	1.00	98.36	A
	1281	OE1	GLN	683	55.147	-5.148	17.678	1.00	99.32	A
	1282	NE2	GLN	683	57.189	-4.835	16.795	1.00	98.03	A
	1283	C	GLN	683	58.425	-6.725	14.029	1.00	94.16	A
40	1284	O	GLN	683	58.599	-5.516	13.948	1.00	94.61	A
	1285	N	GLU	684	59.301	-7.596	13.563	1.00	94.49	A
	1286	CA	GLU	684	60.494	-7.084	12.915	1.00	95.02	A
45	1287	CB	GLU	684	61.445	-8.230	12.567	1.00	97.72	A
	1288	CG	GLU	684	61.936	-9.001	13.790	1.00	101.32	A
	1289	CD	GLU	684	62.713	-10.245	13.404	1.00	104.63	A
	1290	OE1	GLU	684	62.269	-10.940	12.460	1.00	106.64	A
50	1291	OE2	GLU	684	63.753	-10.534	14.043	1.00	105.52	A
	1292	C	GLU	684	60.092	-6.292	11.671	1.00	93.12	A
	1293	O	GLU	684	60.516	-5.148	11.509	1.00	93.19	A
55	1294	N	LEU	685	59.257	-6.893	10.814	1.00	90.38	A
	1295	CA	LEU	685	58.783	-6.237	9.591	1.00	88.13	A

TABLE 2 (continued)

TABLE 2 (continued)									
ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1296	CB	LEU	685	57.904	-7.198	8.760	1.00	87.12	A
1297	CG	LEU	685	58.232	-7.458	7.278	1.00	86.54	A
1298	CD1	LEU	685	56.980	-7.975	6.550	1.00	86.04	A
1299	CD2	LEU	685	58.720	-6.181	6.613	1.00	85.14	A
1300	C	LEU	685	57.970	-4.993	9.975	1.00	87.42	A
1301	O	LEU	685	58.225	-3.894	9.482	1.00	87.78	A
1302	N	PHE	686	56.990	-5.178	10.860	1.00	85.68	A
1303	CA	PHE	686	56.161	-4.083	11.334	1.00	83.88	A
1304	CB	PHE	686	55.399	-4.497	12.587	1.00	82.21	A
1305	CG	PHE	686	54.501	-3.431	13.117	1.00	80.95	A
1306	CD1	PHE	686	53.229	-3.267	12.590	1.00	80.85	A
1307	CD2	PHE	686	54.948	-2.542	14.090	1.00	80.25	A
1308	CE1	PHE	686	52.399	-2.243	13.024	1.00	80.58	A
1309	CE2	PHE	686	54.127	-1.505	14.533	1.00	80.77	A
1310	CZ	PHE	686	52.851	-1.352	13.995	1.00	80.71	A
1311	C	PHE	686	57.013	-2.869	11.693	1.00	84.16	A
1312	O	PHE	686	56.863	-1.787	11.125	1.00	84.35	A
1313	N	ASP	687	57.906	-3.051	12.657	1.00	84.16	A
1314	CA	ASP	687	58.755	-1.955	13.088	1.00	84.15	A
1315	CB	ASP	687	59.742	-2.445	14.165	1.00	86.11	A
1316	CG	ASP	687	59.088	-2.582	15.559	1.00	87.77	A
1317	OD1	ASP	687	59.737	-3.133	16.479	1.00	88.21	A
1318	OD2	ASP	687	57.928	-2.131	15.738	1.00	88.58	A
1319	C	ASP	687	59.476	-1.326	11.895	1.00	83.05	A
1320	O	ASP	687	59.734	-0.123	11.886	1.00	82.98	A
1321	N	GLU	688	59.757	-2.135	10.878	1.00	81.82	A
1322	CA	GLU	688	60.446	-1.684	9.664	1.00	81.05	A
1323	CB	GLU	688	60.962	-2.903	8.894	1.00	84.35	A
1324	CG	GLU	688	62.429	-2.835	8.520	1.00	89.90	A
1325	CD	GLU	688	62.642	-2.602	7.037	1.00	93.24	A
1326	OE1	GLU	688	62.207	-3.464	6.232	1.00	94.85	A
1327	OE2	GLU	688	63.244	-1.557	6.680	1.00	94.38	A
1328	C	GLU	688	59.543	-0.851	8.748	1.00	78.17	A
1329	O	GLU	688	59.974	0.133	8.142	1.00	77.26	A
1330	N	ILE	689	58.290	-1.274	8.628	1.00	74.88	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1331	CA	ILE	689	57.334	-0.562	7.807	1.00	71.74	A
	1332	CB	ILE	689	56.039	-1.363	7.701	1.00	70.89	A
10	1333	CG2	ILE	689	55.087	-0.735	6.694	1.00	70.61	A
	1334	CG1	ILE	689	56.393	-2.772	7.253	1.00	70.37	A
	1335	CD1	ILE	689	55.212	-3.643	7.021	1.00	70.93	A
15	1336	C	ILE	689	57.126	0.753	8.527	1.00	70.52	A
	1337	O	ILE	689	57.470	1.809	8.012	1.00	70.29	A
	1338	N	ARG	690	56.600	0.701	9.745	1.00	68.49	A
	1339	CA	ARG	690	56.413	1.936	10.470	1.00	67.14	A
20	1340	CB	ARG	690	56.263	1.660	11.948	1.00	66.55	A
	1341	CG	ARG	690	55.840	2.865	12.729	1.00	65.66	A
	1342	CD	ARG	690	54.881	2.378	13.767	1.00	66.86	A
25	1343	NE	ARG	690	54.332	3.440	14.589	1.00	69.11	A
	1344	CZ	ARG	690	55.062	4.204	15.386	1.00	71.32	A
	1345	NH1	ARG	690	56.371	4.020	15.458	1.00	71.35	A
	1346	NH2	ARG	690	54.481	5.144	16.123	1.00	72.01	A
30	1347	C	ARG	690	57.566	2.926	10.263	1.00	66.75	A
	1348	O	ARG	690	57.328	4.088	9.972	1.00	66.46	A
	1349	N	MET	691	58.814	2.478	10.398	1.00	67.31	A
35	1350	CA	MET	691	59.941	3.402	10.241	1.00	68.50	A
	1351	CB	MET	691	61.241	2.753	10.733	1.00	70.62	A
	1352	CG	MET	691	62.461	3.684	10.735	1.00	73.77	A
	1353	SD	MET	691	62.232	5.254	11.652	1.00	79.07	A
40	1354	CE	MET	691	61.883	4.634	13.390	1.00	75.73	A
	1355	C	MET	691	60.115	3.933	8.813	1.00	67.84	A
	1356	O	MET	691	60.691	5.005	8.602	1.00	67.23	A
45	1357	N	THR	692	59.617	3.186	7.835	1.00	67.57	A
	1358	CA	THR	692	59.706	3.621	6.452	1.00	66.26	A
	1359	CB	THR	692	59.374	2.483	5.479	1.00	66.50	A
	1360	OG1	THR	692	60.548	1.686	5.260	1.00	67.25	A
50	1361	CG2	THR	692	58.880	3.037	4.162	1.00	66.69	A
	1362	C	THR	692	58.730	4.770	6.255	1.00	65.64	A
	1363	O	THR	692	59.078	5.784	5.642	1.00	65.69	A
55	1364	N	TYR	693	57.513	4.621	6.779	1.00	64.80	A
	1365	CA	TYR	693	56.536	5.701	6.664	1.00	64.71	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1366	CB	TYR	693	55.103	5.201	6.886	1.00	64.94	A
1367	CG	TYR	693	54.677	4.298	5.766	1.00	66.69	A
1368	CD1	TYR	693	54.722	4.748	4.440	1.00	67.11	A
1369	CE1	TYR	693	54.519	3.881	3.386	1.00	67.34	A
1370	CD2	TYR	693	54.393	2.955	6.001	1.00	66.21	A
1371	CE2	TYR	693	54.190	2.078	4.954	1.00	67.07	A
1372	CZ	TYR	693	54.264	2.543	3.647	1.00	68.00	A
1373	OH	TYR	693	54.152	1.651	2.603	1.00	69.03	A
1374	C	TYR	693	56.824	6.877	7.589	1.00	64.42	A
1375	O	TYR	693	56.325	7.969	7.344	1.00	65.00	A
1376	N	ILE	694	57.605	6.694	8.650	1.00	63.88	A
1377	CA	ILE	694	57.900	7.859	9.472	1.00	62.99	A
1378	CB	ILE	694	58.571	7.515	10.821	1.00	62.36	A
1379	CG2	ILE	694	59.061	8.789	11.501	1.00	61.36	A
1380	CG1	ILE	694	57.553	6.852	11.746	1.00	62.16	A
1381	CD1	ILE	694	58.137	6.409	13.056	1.00	61.49	A
1382	C	ILE	694	58.853	8.701	8.640	1.00	62.62	A
1383	O	ILE	694	58.890	9.919	8.757	1.00	62.37	A
1384	N	LYS	695	59.611	8.042	7.773	1.00	63.30	A
1385	CA	LYS	695	60.541	8.761	6.924	1.00	64.01	A
1386	CB	LYS	695	61.656	7.820	6.452	1.00	65.96	A
1387	CG	LYS	695	62.589	7.316	7.569	1.00	68.75	A
1388	CD	LYS	695	63.633	6.371	6.975	1.00	71.84	A
1389	CE	LYS	695	64.652	5.841	7.993	1.00	74.93	A
1390	NZ	LYS	695	65.646	4.889	7.367	1.00	75.72	A
1391	C	LYS	695	59.804	9.390	5.733	1.00	63.18	A
1392	O	LYS	695	60.101	10.514	5.335	1.00	63.38	A
1393	N	GLU	696	58.837	8.671	5.177	1.00	62.48	A
1394	CA	GLU	696	58.059	9.179	4.058	1.00	62.80	A
1395	CB	GLU	696	56.969	8.156	3.715	1.00	62.84	A
1396	CG	GLU	696	56.901	7.590	2.268	1.00	65.44	A
1397	CD	GLU	696	57.947	8.126	1.269	1.00	68.55	A
1398	OE1	GLU	696	59.132	7.725	1.358	1.00	69.98	A
1399	OE2	GLU	696	57.574	8.933	0.380	1.00	69.05	A
1400	C	GLU	696	57.442	10.532	4.494	1.00	63.48	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1401	O	GLU	696	57.417	11.494	3.721	1.00	63.32	A
	1402	N	LEU	697	56.960	10.593	5.743	1.00	63.97	A
10	1403	CA	LEU	697	56.350	11.799	6.336	1.00	63.42	A
	1404	CB	LEU	697	55.832	11.516	7.764	1.00	62.28	A
	1405	CG	LEU	697	55.230	12.693	8.555	1.00	61.21	A
15	1406	CD1	LEU	697	53.962	13.141	7.867	1.00	59.88	A
	1407	CD2	LEU	697	54.919	12.305	10.000	1.00	61.08	A
	1408	C	LEU	697	57.360	12.939	6.401	1.00	63.31	A
	1409	O	LEU	697	57.017	14.101	6.195	1.00	63.33	A
20	1410	N	GLY	698	58.604	12.604	6.708	1.00	63.85	A
	1411	CA	GLY	698	59.631	13.623	6.771	1.00	64.63	A
	1412	C	GLY	698	59.873	14.137	5.370	1.00	65.37	A
25	1413	O	GLY	698	60.160	15.311	5.164	1.00	65.08	A
	1414	N	LYS	699	59.754	13.247	4.394	1.00	66.39	A
	1415	CA	LYS	699	59.947	13.649	3.011	1.00	68.06	A
	1416	CB	LYS	699	59.919	12.437	2.109	1.00	68.79	A
30	1417	CG	LYS	699	61.185	11.646	2.136	1.00	71.18	A
	1418	CD	LYS	699	60.963	10.397	1.352	1.00	71.92	A
	1419	CE	LYS	699	62.237	9.864	0.785	1.00	72.64	A
35	1420	NZ	LYS	699	61.851	8.836	-0.208	1.00	73.27	A
	1421	C	LYS	699	58.845	14.604	2.604	1.00	69.09	A
	1422	O	LYS	699	59.098	15.610	1.933	1.00	69.42	A
40	1423	N	ALA	700	57.620	14.277	3.011	1.00	68.96	A
	1424	CA	ALA	700	56.471	15.105	2.711	1.00	68.91	A
	1425	CB	ALA	700	55.235	14.525	3.356	1.00	68.39	A
	1426	C	ALA	700	56.747	16.496	3.250	1.00	70.45	A
45	1427	O	ALA	700	56.729	17.464	2.500	1.00	70.63	A
	1428	N	ILE	701	57.017	16.581	4.556	1.00	72.26	A
	1429	CA	ILE	701	57.319	17.847	5.249	1.00	74.11	A
50	1430	CB	ILE	701	57.961	17.556	6.637	1.00	72.88	A
	1431	CG2	ILE	701	58.462	18.835	7.280	1.00	71.61	A
	1432	CG1	ILE	701	56.943	16.850	7.529	1.00	72.83	A
	1433	CD1	ILE	701	57.216	16.974	9.009	1.00	72.05	A
55	1434	C	ILE	701	58.282	18.721	4.445	1.00	76.37	A
	1435	O	ILE	701	57.977	19.860	4.077	1.00	75.84	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1436	N	VAL	702	59.453	18.162	4.193	1.00	79.02	A
1437	CA	VAL	702	60.505	18.815	3.441	1.00	83.18	A
1438	CB	VAL	702	61.653	17.827	3.195	1.00	83.12	A
1439	CG1	VAL	702	62.631	18.405	2.202	1.00	83.67	A
1440	CG2	VAL	702	62.348	17.502	4.507	1.00	82.28	A
1441	C	VAL	702	60.052	19.381	2.094	1.00	85.97	A
1442	O	VAL	702	60.257	20.561	1.813	1.00	86.89	A
1443	N	LYS	703	59.466	18.527	1.262	1.00	89.29	A
1444	CA	LYS	703	58.980	18.906	-0.070	1.00	92.79	A
1445	CB	LYS	703	58.138	17.740	-0.638	1.00	90.47	A
1446	CG	LYS	703	58.014	17.642	-2.173	1.00	89.42	A
1447	CD	LYS	703	57.321	16.325	-2.633	1.00	88.53	A
1448	CE	LYS	703	57.388	16.120	-4.166	1.00	87.74	A
1449	NZ	LYS	703	56.350	15.184	-4.728	1.00	87.46	A
1450	C	LYS	703	58.139	20.197	0.041	1.00	96.58	A
1451	O	LYS	703	58.300	21.149	-0.738	1.00	96.91	A
1452	N	ARG	704	57.266	20.194	1.047	1.00	100.79	A
1453	CA	ARG	704	56.327	21.260	1.393	1.00	104.87	A
1454	CB	ARG	704	55.784	20.985	2.806	1.00	105.73	A
1455	CG	ARG	704	54.977	22.104	3.412	1.00	107.49	A
1456	CD	ARG	704	54.209	21.704	4.659	1.00	109.11	A
1457	NE	ARG	704	53.494	22.890	5.106	1.00	111.38	A
1458	CZ	ARG	704	54.049	23.883	5.794	1.00	112.38	A
1459	NH1	ARG	704	55.331	23.825	6.150	1.00	112.57	A
1460	NH2	ARG	704	53.349	24.978	6.055	1.00	112.76	A
1461	C	ARG	704	56.906	22.651	1.359	1.00	107.58	A
1462	O	ARG	704	56.307	23.618	0.874	1.00	108.13	A
1463	N	GLU	705	58.102	22.745	1.878	1.00	110.53	A
1464	CA	GLU	705	58.710	24.028	1.971	1.00	113.44	A
1465	CB	GLU	705	58.866	24.321	3.440	1.00	114.43	A
1466	CG	GLU	705	59.182	23.034	4.168	1.00	115.34	A
1467	CD	GLU	705	59.016	23.153	5.646	1.00	116.03	A
1468	OE1	GLU	705	59.832	23.860	6.269	1.00	116.67	A
1469	OE2	GLU	705	58.065	22.547	6.184	1.00	116.66	A
1470	C	GLU	705	60.034	24.037	1.301	1.00	114.62	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1471	O	GLU	705	60.574	23.003	0.902	1.00	114.77	A
	1472	N	GLY	706	60.543	25.241	1.152	1.00	116.18	A
10	1473	CA	GLY	706	61.852	25.398	0.588	1.00	118.63	A
	1474	C	GLY	706	62.672	25.661	1.834	1.00	120.26	A
	1475	O	GLY	706	63.853	25.330	1.897	1.00	121.20	A
15	1476	N	ASN	707	62.000	26.216	2.845	1.00	120.91	A
	1477	CA	ASN	707	62.581	26.609	4.137	1.00	121.19	A
	1478	CB	ASN	707	61.710	27.710	4.716	1.00	122.25	A
	1479	CG	ASN	707	60.240	27.387	4.585	1.00	123.17	A
20	1480	OD1	ASN	707	59.792	26.332	5.026	1.00	123.06	A
	1481	ND2	ASN	707	59.481	28.285	3.963	1.00	123.82	A
	1482	C	ASN	707	62.791	25.529	5.210	1.00	120.52	A
25	1483	O	ASN	707	61.919	25.294	6.052	1.00	120.14	A
	1484	N	SER	708	63.978	24.927	5.197	1.00	120.09	A
	1485	CA	SER	708	64.367	23.864	6.126	1.00	119.78	A
	1486	CB	SER	708	65.610	23.146	5.586	1.00	120.58	A
30	1487	OG	SER	708	65.402	22.691	4.257	1.00	121.41	A
	1488	C	SER	708	64.639	24.344	7.555	1.00	118.82	A
	1489	O	SER	708	65.222	23.619	8.368	1.00	118.32	A
35	1490	N	SER	709	64.208	25.565	7.850	1.00	117.85	A
	1491	CA	SER	709	64.394	26.147	9.174	1.00	116.73	A
	1492	CB	SER	709	64.188	27.660	9.091	1.00	117.22	A
	1493	OG	SER	709	65.042	28.217	8.105	1.00	118.10	A
40	1494	C	SER	709	63.429	25.517	10.191	1.00	115.52	A
	1495	O	SER	709	63.830	25.193	11.317	1.00	115.87	A
	1496	N	GLN	710	62.168	25.339	9.791	1.00	112.97	A
45	1497	CA	GLN	710	61.169	24.729	10.669	1.00	109.62	A
	1498	CB	GLN	710	59.958	25.657	10.849	1.00	111.67	A
	1499	CG	GLN	710	60.193	26.759	11.894	1.00	113.15	A
50	1500	CD	GLN	710	58.910	27.387	12.420	1.00	114.64	A
	1501	OE1	GLN	710	58.939	28.182	13.364	1.00	115.78	A
	1502	NE2	GLN	710	57.776	27.035	11.815	1.00	114.86	A
	1503	C	GLN	710	60.720	23.340	10.198	1.00	106.11	A
55	1504	O	GLN	710	59.542	22.973	10.293	1.00	105.36	A
	1505	N	ASN	711	61.682	22.573	9.692	1.00	101.53	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
10	1506	CA	ASN	711	61.406	21.225	9.242	1.00	96.35	A
	1507	CB	ASN	711	62.540	20.705	8.362	1.00	95.93	A
	1508	CG	ASN	711	62.287	20.980	6.892	1.00	96.22	A
	1509	OD1	ASN	711	63.138	20.721	6.041	1.00	96.50	A
	1510	ND2	ASN	711	61.101	21.502	6.587	1.00	95.88	A
15	1511	C	ASN	711	61.200	20.339	10.461	1.00	93.06	A
	1512	O	ASN	711	60.173	19.673	10.568	1.00	92.98	A
	1513	N	TRP	712	62.142	20.328	11.395	1.00	88.90	A
20	1514	CA	TRP	712	61.896	19.508	12.573	1.00	85.12	A
	1515	CB	TRP	712	63.139	19.345	13.448	1.00	82.71	A
	1516	CG	TRP	712	64.206	18.565	12.816	1.00	78.88	A
	1517	CD2	TRP	712	64.273	17.140	12.692	1.00	77.30	A
25	1518	CE2	TRP	712	65.454	16.845	11.979	1.00	77.10	A
	1519	CE3	TRP	712	63.495	16.079	13.175	1.00	76.79	A
	1520	CD1	TRP	712	65.278	19.061	12.155	1.00	77.85	A
30	1521	NE1	TRP	712	66.032	18.038	11.638	1.00	77.39	A
	1522	CZ2	TRP	712	65.824	15.539	11.650	1.00	77.27	A
	1523	CZ3	TRP	712	63.869	14.773	12.857	1.00	77.22	A
	1524	CH2	TRP	712	65.043	14.516	12.126	1.00	76.39	A
35	1525	C	TRP	712	60.781	20.095	13.427	1.00	84.16	A
	1526	O	TRP	712	60.240	19.394	14.280	1.00	84.15	A
	1527	N	GLN	713	60.426	21.359	13.233	1.00	83.31	A
40	1528	CA	GLN	713	59.352	21.887	14.059	1.00	82.44	A
	1529	CB	GLN	713	59.316	23.418	14.051	1.00	85.53	A
	1530	CG	GLN	713	58.358	24.025	15.110	1.00	89.96	A
	1531	CD	GLN	713	58.571	23.473	16.534	1.00	92.69	A
45	1532	OE1	GLN	713	57.728	22.737	17.066	1.00	92.02	A
	1533	NE2	GLN	713	59.701	23.832	17.152	1.00	93.58	A
	1534	C	GLN	713	58.014	21.327	13.595	1.00	80.69	A
50	1535	O	GLN	713	57.169	20.991	14.417	1.00	80.26	A
	1536	N	ARG	714	57.840	21.202	12.281	1.00	78.63	A
	1537	CA	ARG	714	56.596	20.673	11.715	1.00	76.05	A
55	1538	CB	ARG	714	56.511	20.977	10.226	1.00	75.18	A
	1539	CG	ARG	714	55.148	20.658	9.665	1.00	74.15	A
	1540	CD	ARG	714	55.015	21.162	8.264	1.00	73.11	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1541	NE	ARG	714	53.718	20.828	7.681	1.00	72.23	A
	1542	CZ	ARG	714	52.573	21.419	8.001	1.00	71.10	A
10	1543	NH1	ARG	714	52.542	22.374	8.917	1.00	70.94	A
	1544	NH2	ARG	714	51.459	21.068	7.372	1.00	69.74	A
	1545	C	ARG	714	56.448	19.173	11.918	1.00	75.24	A
15	1546	O	ARG	714	55.332	18.655	12.017	1.00	75.01	A
	1547	N	PHE	715	57.573	18.475	11.953	1.00	74.26	A
	1548	CA	PHE	715	57.544	17.043	12.167	1.00	73.79	A
	1549	CB	PHE	715	58.935	16.456	12.019	1.00	73.23	A
20	1550	CG	PHE	715	58.969	14.973	12.143	1.00	73.54	A
	1551	CD1	PHE	715	58.715	14.169	11.038	1.00	74.69	A
	1552	CD2	PHE	715	59.213	14.372	13.367	1.00	74.25	A
25	1553	CE1	PHE	715	58.720	12.791	11.148	1.00	74.64	A
	1554	CE2	PHE	715	59.219	12.990	13.494	1.00	74.97	A
	1555	CZ	PHE	715	58.968	12.196	12.383	1.00	75.12	A
	1556	C	PHE	715	57.049	16.804	13.586	1.00	73.88	A
30	1557	O	PHE	715	56.413	15.791	13.875	1.00	73.98	A
	1558	N	TYR	716	57.356	17.756	14.466	1.00	74.00	A
	1559	CA	TYR	716	56.950	17.682	15.862	1.00	73.76	A
35	1560	CB	TYR	716	57.698	18.738	16.681	1.00	74.90	A
	1561	CG	TYR	716	57.303	18.724	18.134	1.00	76.12	A
	1562	CD1	TYR	716	57.656	17.657	18.961	1.00	76.63	A
	1563	CE1	TYR	716	57.199	17.579	20.270	1.00	77.14	A
40	1564	CD2	TYR	716	56.493	19.725	18.659	1.00	76.34	A
	1565	CE2	TYR	716	56.028	19.657	19.964	1.00	77.79	A
	1566	CZ	TYR	716	56.383	18.581	20.764	1.00	77.71	A
45	1567	OH	TYR	716	55.878	18.483	22.037	1.00	77.98	A
	1568	C	TYR	716	55.445	17.900	16.008	1.00	73.41	A
	1569	O	TYR	716	54.773	17.154	16.720	1.00	73.40	A
50	1570	N	GLN	717	54.932	18.930	15.341	1.00	72.86	A
	1571	CA	GLN	717	53.506	19.246	15.381	1.00	72.51	A
	1572	CB	GLN	717	53.199	20.517	14.570	1.00	74.03	A
	1573	CG	GLN	717	53.717	21.832	15.172	1.00	77.70	A
55	1574	CD	GLN	717	53.451	23.065	14.288	1.00	80.63	A
	1575	OE1	GLN	717	53.797	23.094	13.098	1.00	81.29	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1576	NE2	GLN	717	52.848	24.096	14.881	1.00	81.96	A
1577	C	GLN	717	52.728	18.074	14.791	1.00	71.31	A
1578	O	GLN	717	51.828	17.516	15.418	1.00	71.30	A
1579	N	LEU	718	53.089	17.687	13.575	1.00	68.89	A
1580	CA	LEU	718	52.396	16.596	12.931	1.00	66.70	A
1581	CB	LEU	718	53.019	16.309	11.578	1.00	65.16	A
1582	CG	LEU	718	52.851	17.456	10.603	1.00	64.70	A
1583	CD1	LEU	718	53.411	17.030	9.276	1.00	64.31	A
1584	CD2	LEU	718	51.387	17.819	10.472	1.00	65.25	A
1585	C	LEU	718	52.322	15.303	13.717	1.00	66.09	A
1586	O	LEU	718	51.271	14.677	13.761	1.00	66.32	A
1587	N	THR	719	53.429	14.894	14.331	1.00	66.23	A
1588	CA	THR	719	53.441	13.637	15.074	1.00	67.26	A
1589	CB	THR	719	54.880	13.161	15.289	1.00	67.26	A
1590	OG1	THR	719	55.556	14.070	16.161	1.00	67.19	A
1591	CG2	THR	719	55.618	13.100	13.947	1.00	65.43	A
1592	C	THR	719	52.715	13.758	16.417	1.00	68.33	A
1593	O	THR	719	52.254	12.758	16.995	1.00	67.95	A
1594	N	LYS	720	52.623	15.003	16.885	1.00	69.49	A
1595	CA	LYS	720	51.937	15.361	18.120	1.00	70.54	A
1596	CB	LYS	720	52.232	16.839	18.424	1.00	73.28	A
1597	CG	LYS	720	52.196	17.259	19.894	1.00	77.37	A
1598	CD	LYS	720	53.224	16.488	20.738	1.00	80.58	A
1599	CE	LYS	720	52.565	15.638	21.853	1.00	82.40	A
1600	NZ	LYS	720	51.608	14.564	21.400	1.00	81.87	A
1601	C	LYS	720	50.438	15.137	17.809	1.00	69.73	A
1602	O	LYS	720	49.680	14.604	18.629	1.00	70.78	A
1603	N	LEU	721	50.029	15.530	16.599	1.00	67.65	A
1604	CA	LEU	721	48.649	15.353	16.146	1.00	65.04	A
1605	CB	LEU	721	48.450	15.934	14.740	1.00	63.50	A
1606	CG	LEU	721	47.028	16.423	14.419	1.00	62.27	A
1607	CD1	LEU	721	46.820	16.517	12.919	1.00	60.98	A
1608	CD2	LEU	721	46.008	15.489	15.027	1.00	62.51	A
1609	C	LEU	721	48.348	13.860	16.093	1.00	64.45	A
1610	O	LEU	721	47.318	13.407	16.581	1.00	65.22	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1611	N	LEU	722	49.249	13.108	15.467	1.00	63.64	A
	1612	CA	LEU	722	49.095	11.668	15.344	1.00	62.92	A
10	1613	CB	LEU	722	50.359	11.048	14.764	1.00	60.54	A
	1614	CG	LEU	722	50.490	11.222	13.260	1.00	57.75	A
	1615	CD1	LEU	722	51.771	10.603	12.779	1.00	55.67	A
15	1616	CD2	LEU	722	49.301	10.577	12.589	1.00	55.86	A
	1617	C	LEU	722	48.832	11.061	16.695	1.00	64.43	A
	1618	O	LEU	722	47.985	10.175	16.833	1.00	64.56	A
	1619	N	ASP	723	49.575	11.544	17.689	1.00	66.00	A
20	1620	CA	ASP	723	49.440	11.071	19.063	1.00	67.32	A
	1621	CB	ASP	723	50.504	11.708	19.957	1.00	68.83	A
	1622	CG	ASP	723	51.815	10.946	19.958	1.00	71.08	A
25	1623	OD1	ASP	723	51.917	9.887	19.293	1.00	71.58	A
	1624	OD2	ASP	723	52.751	11.416	20.646	1.00	72.22	A
	1625	C	ASP	723	48.061	11.390	19.635	1.00	67.50	A
	1626	O	ASP	723	47.419	10.530	20.233	1.00	67.38	A
30	1627	N	SER	724	47.605	12.622	19.460	1.00	67.60	A
	1628	CA	SER	724	46.306	12.979	19.998	1.00	68.26	A
	1629	CB	SER	724	46.055	14.481	19.846	1.00	69.65	A
35	1630	OG	SER	724	46.043	14.873	18.485	1.00	72.65	A
	1631	C	SER	724	45.170	12.186	19.355	1.00	68.41	A
	1632	O	SER	724	44.018	12.323	19.749	1.00	68.56	A
	1633	N	MET	725	45.477	11.354	18.361	1.00	68.11	A
40	1634	CA	MET	725	44.421	10.567	17.737	1.00	66.74	A
	1635	CB	MET	725	44.856	10.002	16.384	1.00	65.02	A
	1636	CG	MET	725	44.938	11.011	15.260	1.00	63.01	A
45	1637	SD	MET	725	43.372	11.815	14.850	1.00	61.30	A
	1638	CE	MET	725	42.296	10.467	14.601	1.00	60.48	A
	1639	C	MET	725	44.038	9.417	18.650	1.00	67.46	A
	1640	O	MET	725	42.928	8.894	18.555	1.00	68.23	A
50	1641	N	HIS	726	44.948	9.000	19.524	1.00	67.20	A
	1642	CA	HIS	726	44.596	7.924	20.433	1.00	67.38	A
	1643	CB	HIS	726	45.810	7.409	21.227	1.00	64.41	A
55	1644	CG	HIS	726	46.804	6.622	20.417	1.00	60.65	A
	1645	CD2	HIS	726	48.071	6.926	20.043	1.00	59.49	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1646	ND1	HIS	726	46.566	5.346	19.969	1.00	59.00	A
1647	CE1	HIS	726	47.649	4.886	19.352	1.00	58.49	A
1648	NE2	HIS	726	48.571	5.825	19.385	1.00	58.18	A
1649	C	HIS	726	43.563	8.519	21.389	1.00	69.98	A
1650	O	HIS	726	42.660	7.820	21.825	1.00	71.06	A
1651	N	GLU	727	43.679	9.811	21.704	1.00	73.24	A
1652	CA	GLU	727	42.711	10.453	22.604	1.00	76.05	A
1653	CB	GLU	727	43.221	11.847	23.070	1.00	78.51	A
1654	CG	GLU	727	43.221	11.847	23.070	1.00	78.51	A
1655	CD	GLU	727	42.424	13.114	22.613	1.00	84.07	A
1656	OE1	GLU	727	42.424	13.114	22.613	1.00	84.07	A
1657	OE2	GLU	727	44.458	14.402	22.987	1.00	87.46	A
1658	C	GLU	727	44.458	14.402	22.987	1.00	87.46	A
1659	O	GLU	727	42.829	15.406	21.901	1.00	88.22	A
1660	N	VAL	728	42.829	15.406	21.901	1.00	87.58	A
1661	CA	VAL	728	41.345	10.570	21.935	1.00	76.51	A
1662	CB	VAL	728	41.345	10.570	21.935	1.00	76.51	A
1663	CG1	VAL	728	40.334	10.193	22.520	1.00	76.62	A
1664	CG2	VAL	728	40.334	10.193	22.520	1.00	76.62	A
1665	C	VAL	728	41.287	11.059	20.705	1.00	77.36	A
1666	O	VAL	728	41.287	11.059	20.705	1.00	77.36	A
1667	N	VAL	729	39.977	11.185	20.094	1.00	77.61	A
1668	CA	VAL	729	39.977	11.185	20.094	1.00	77.61	A
1669	CB	VAL	729	39.992	12.131	18.867	1.00	77.17	A
1670	CG1	VAL	729	39.992	12.131	18.867	1.00	77.17	A
1671	CG2	VAL	729	41.342	12.768	18.725	1.00	77.42	A
1672	C	VAL	729	41.342	12.768	18.725	1.00	77.42	A
1673	O	VAL	729	41.342	12.768	18.725	1.00	77.42	A
1674	N	GLU	730	39.603	11.395	17.614	1.00	77.94	A
1675	CA	GLU	730	39.603	11.395	17.614	1.00	77.94	A
1676	CB	GLU	730	39.371	9.829	19.740	1.00	78.18	A
1677	CG	GLU	730	39.371	9.829	19.740	1.00	78.18	A
1678	CD	GLU	730	38.155	9.655	19.855	1.00	78.24	A
1679	OE1	GLU	730	38.155	9.655	19.855	1.00	78.24	A
1680	OE2	GLU	730	40.188	8.864	19.325	1.00	79.36	A
				40.188	8.864	19.325	1.00	79.36	A
				39.628	7.555	19.008	1.00	80.65	A
				39.628	7.555	19.008	1.00	80.65	A
				40.693	6.546	18.563	1.00	80.37	A
				40.693	6.546	18.563	1.00	80.37	A
				40.092	5.154	18.530	1.00	80.54	A
				40.092	5.154	18.530	1.00	80.54	A
				41.194	6.905	17.183	1.00	81.12	A
				41.194	6.905	17.183	1.00	81.12	A
				38.950	7.020	20.259	1.00	81.61	A
				38.950	7.020	20.259	1.00	81.61	A
				37.795	6.606	20.220	1.00	82.29	A
				37.795	6.606	20.220	1.00	82.29	A
				39.672	7.029	21.369	1.00	82.79	A
				39.672	7.029	21.369	1.00	82.79	A
				39.101	6.566	22.620	1.00	84.17	A
				39.101	6.566	22.620	1.00	84.17	A
				40.008	7.016	23.754	1.00	85.48	A
				40.008	7.016	23.754	1.00	85.48	A
				39.686	6.476	25.117	1.00	88.56	A
				39.686	6.476	25.117	1.00	88.56	A
				40.765	6.857	26.102	1.00	90.50	A
				40.765	6.857	26.102	1.00	90.50	A
				41.174	8.040	26.096	1.00	91.35	A
				41.174	8.040	26.096	1.00	91.35	A
				41.207	5.982	26.876	1.00	92.37	A
				41.207	5.982	26.876	1.00	92.37	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1681	C	GLU	730	37.671	7.137	22.766	1.00	84.44	A
	1682	O	GLU	730	36.709	6.375	22.882	1.00	84.46	A
10	1683	N	ASN	731	37.529	8.462	22.726	1.00	85.16	A
	1684	CA	ASN	731	36.214	9.114	22.839	1.00	85.37	A
	1685	CB	ASN	731	36.325	10.622	22.682	1.00	86.19	A
15	1686	CG	ASN	731	36.897	11.274	23.882	1.00	86.88	A
	1687	OD1	ASN	731	36.493	10.986	25.005	1.00	88.09	A
	1688	ND2	ASN	731	37.840	12.177	23.667	1.00	87.13	A
	1689	C	ASN	731	35.213	8.666	21.803	1.00	85.12	A
20	1690	O	ASN	731	34.036	8.481	22.102	1.00	84.67	A
	1691	N	LEU	732	35.676	8.545	20.573	1.00	84.94	A
	1692	CA	LEU	732	34.789	8.139	19.511	1.00	85.15	A
25	1693	CB	LEU	732	35.490	8.262	18.167	1.00	83.41	A
	1694	CG	LEU	732	35.707	9.696	17.691	1.00	82.65	A
	1695	CD1	LEU	732	36.028	9.661	16.211	1.00	82.43	A
	1696	CD2	LEU	732	34.458	10.530	17.939	1.00	81.93	A
30	1697	C	LEU	732	34.269	6.727	19.718	1.00	86.42	A
	1698	O	LEU	732	33.076	6.476	19.564	1.00	85.99	A
	1699	N	LEU	733	35.165	5.818	20.099	1.00	88.47	A
35	1700	CA	LEU	733	34.834	4.407	20.310	1.00	90.36	A
	1701	CB	LEU	733	36.145	3.619	20.442	1.00	89.51	A
	1702	CG	LEU	733	36.535	2.352	19.657	1.00	89.28	A
	1703	CD1	LEU	733	35.949	2.280	18.252	1.00	88.11	A
40	1704	CD2	LEU	733	38.058	2.351	19.600	1.00	88.74	A
	1705	C	LEU	733	33.886	4.098	21.488	1.00	92.45	A
	1706	O	LEU	733	32.949	3.309	21.325	1.00	92.88	A
45	1707	N	ASN	734	34.111 1	4.699	22.662	1.00	94.41	A
	1708	CA	ASN	734	33.239	4.446	23.826	1.00	96.34	A
	1709	CB	ASN	734	33.569	5.380	24.990	1.00	98.01	A
	1710	CG	ASN	734	34.943	5.145	25.555	1.00	100.48	A
50	1711	OD1	ASN	734	35.434	4.013	25.576	1.00	101.32	A
	1712	ND2	ASN	734	35.571	6.209	26.039	1.00	101.67	A
	1713	C	ASN	734	31.785	4.673	23.465	1.00	96.76	A
55	1714	O	ASN	734	30.903	3.870	23.769	1.00	96.85	A
	1715	N	TYR	735	31.568	5.817	22.828	1.00	97.87	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1716	CA	TYR	735	30.272	6.279	22.366	1.00	98.53	A
1717	CB	TYR	735	30.446	7.677	21.791	1.00	100.86	A
1718	CG	TYR	735	29.259	8.590	21.899	1.00	103.46	A
1719	CD1	TYR	735	27.960	8.131	21.665	1.00	104.41	A
1720	CE1	TYR	735	26.864	8.992	21.773	1.00	106.25	A
1721	CD2	TYR	735	29.445	9.927	22.244	1.00	104.91	A
1722	CE2	TYR	735	28.374	10.799	22.357	1.00	106.48	A
1723	CZ	TYR	735	27.081	10.331	22.119	1.00	107.25	A
1724	OH	TYR	735	26.037	11.228	22.198	1.00	108.22	A
1725	C	TYR	735	29.767	5.363	21.258	1.00	97.72	A
1726	O	TYR	735	28.607	5.437	20.856	1.00	98.21	A
1727	N	CYS	736	30.652	4.519	20.744	1.00	96.14	A
1728	CA	CYS	736	30.293	3.611	19.666	1.00	94.51	A
1729	CB	CYS	736	31.473	3.426	18.719	1.00	93.20	A
1730	SG	CYS	736	31.103	2.373	17.310	1.00	89.33	A
1731	C	CYS	736	29.884	2.268	20.225	1.00	94.66	A
1732	O	CYS	736	28.961	1.629	19.719	1.00	93.86	A
1733	N	PHE	737	30.605	1.849	21.262	1.00	95.33	A
1734	CA	PHE	737	30.339	0.596	21.952	1.00	96.63	A
1735	CB	PHE	737	31.484	0.264	22.928	1.00	95.49	A
1736	CG	PHE	737	32.804	-0.094	22.260	1.00	94.69	A
1737	CD1	PHE	737	32.864	-0.453	20.917	1.00	94.73	A
1738	CD2	PHE	737	33.984	-0.136	23.011	1.00	94.55	A
1739	CE1	PHE	737	34.076	-0.846	20.323	1.00	94.35	A
1740	CE2	PHE	737	35.203	-0.528	22.428	1.00	94.76	A
1741	CZ	PHE	737	35.247	-0.885	21.083	1.00	94.34	A
1742	C	PHE	737	29.034	0.811	22.732	1.00	98.44	A
1743	O	PHE	737	28.105	0.003	22.647	1.00	98.71	A
1744	N	GLN	738	28.978	1.917	23.474	1.00	100.30	A
1745	CA	GLN	738	27.801	2.279	24.269	1.00	102.02	A
1746	CB	GLN	738	27.975	3.716	24.854	1.00	102.80	A
1747	CG	GLN	738	27.106	4.083	26.120	1.00	103.60	A
1748	CD	GLN	738	27.583	5.347	26.908	1.00	104.17	A
1749	OE1	GLN	738	26.990	6.429	26.806	1.00	104.86	A
1750	NE2	GLN	738	28.649	5.190	27.697	1.00	104.42	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1751	C	GLN	738	26.573	2.160	23.346	1.00	103.16	A
	1752	O	GLN	738	25.699	1.328	23.592	1.00	103.35	A
10	1753	N	THR	739	26.519	2.936	22.268	1.00	104.30	A
	1754	CA	THR	739	25.366	2.839	21.377	1.00	105.68	A
	1755	CB	THR	739	25.511	3.778	20.162	1.00	105.48	A
15	1756	OG1	THR	739	25.991	5.052	20.613	1.00	106.89	A
	1757	CG2	THR	739	24.153	3.998	19.494	1.00	105.18	A
	1758	C	THR	739	25.164	1.375	20.940	1.00	106.67	A
	1759	O	THR	739	24.187	0.754	21.346	1.00	107.32	A
20	1760	N	PHE	740	26.085	0.808	20.161	1.00	107.75	A
	1761	CA	PHE	740	25.950	-0.590	19.719	1.00	108.45	A
	1762	CB	PHE	740	27.286	-1.127	19.209	1.00	108.59	A
25	1763	CG	PHE	740	27.268	-2.597	18.882	1.00	108.29	A
	1764	CD1	PHE	740	26.881	-3.041	17.620	1.00	108.66	A
	1765	CD2	PHE	740	27.671	-3.534	19.826	1.00	108.06	A
	1766	CE1	PHE	740	26.896	-4.404	17.307	1.00	108.89	A
30	1767	CE2	PHE	740	27.689	-4.898	19.524	1.00	108.14	A
	1768	CZ	PHE	740	27.306	-5.332	18.261	1.00	108.57	A
	1769	C	PHE	740	25.428	-1.560	20.785	1.00	108.81	A
35	1770	O	PHE	740	24.731	-2.519	20.468	1.00	108.65	A
	1771	N	LEU	741	25.797	-1.336	22.042	1.00	109.39	A
	1772	CA	LEU	741	25.322	-2.207	23.108	1.00	110.49	A
	1773	CB	LEU	741	26.425	-2.500	24.115	1.00	109.37	A
40	1774	CG	LEU	741	27.685	-3.170	23.590	1.00	108.46	A
	1775	CD1	LEU	741	28.582	-3.425	24.770	1.00	108.19	A
	1776	CD2	LEU	741	27.365	-4.469	22.876	1.00	108.56	A
45	1777	C	LEU	741	24.182	-1.518	23.822	1.00	112.02	A
	1778	O	LEU	741	24.322	-1.081	24.963	1.00	112.34	A
	1779	N	ASP	742	23.056	-1.419	23.128	1.00	113.82	A
	1780	CA	ASP	742	21.864	-0.782	23.665	1.00	115.47	A
50	1781	CB	ASP	742	22.182	0.625	24.156	1.00	116.03	A
	1782	CG	ASP	742	20.959	1.333	24.685	1.00	117.14	A
	1783	OD1	ASP	742	21.000	2.572	24.835	1.00	117.82	A
55	1784	OD2	ASP	742	19.954	0.643	24.954	1.00	117.31	A
	1785	C	ASP	742	20.805	-0.706	22.575	1.00	116.45	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1786	O	ASP	742	20.649	0.323	21.916	1.00	116.14	A
1787	N	LYS	743	20.084	-1.810	22.392	1.00	118.04	A
1788	CA	LYS	743	19.032	-1.910	21.386	1.00	119.53	A
1789	CB	LYS	743	18.431	-3.330	21.389	1.00	120.38	A
1790	CG	LYS	743	18.709	-4.182	20.127	1.00	121.19	A
1791	CD	LYS	743	18.195	-3.494	18.848	1.00	121.91	A
1792	CE	LYS	743	18.211	-4.400	17.597	1.00	122.04	A
1793	NZ	LYS	743	16.987	-5.256	17.431	1.00	122.03	A
1794	C	LYS	743	17.930	-0.876	21.627	1.00	119.72	A
1795	O	LYS	743	17.253	-0.451	20.688	1.00	119.76	A
1796	N	THR	744	17.758	-0.472	22.883	1.00	120.14	A
1797	CA	THR	744	16.744	0.516	23.243	1.00	120.66	A
1798	CB	THR	744	16.883	0.942	24.736	1.00	120.95	A
1799	OG1	THR	744	17.456	-0.137	25.488	1.00	121.58	A
1800	CG2	THR	744	15.515	1.266	25.333	1.00	120.72	A
1801	C	THR	744	16.910	1.748	22.342	1.00	120.72	A
1802	O	THR	744	15.952	2.489	22.106	1.00	121.13	A
1803	N	MET	745	18.124	1.947	21.835	1.00	120.51	A
1804	CA	MET	745	18.434	3.075	20.950	1.00	119.90	A
1805	CB	MET	745	19.936	3.371	20.968	1.00	120.29	A
1806	CG	MET	745	20.316	4.645	21.706	1.00	120.44	A
1807	SD	MET	745	22.034	4.572	22.232	1.00	121.93	A
1808	CE	MET	745	21.949	5.228	23.955	1.00	121.39	A
1809	C	MET	745	17.988	2.794	19.520	1.00	118.93	A
1810	O	MET	745	17.574	3.701	18.800	1.00	119.40	A
1811	N	SER	746	18.093	1.537	19.109	1.00	117.59	A
1812	CA	SER	746	17.665	1.146	17.776	1.00	116.37	A
1813	CB	SER	746	16.156	1.302	17.664	1.00	116.67	A
1814	OG	SER	746	15.513	0.352	18.490	1.00	117.32	A
1815	C	SER	746	18.342	1.886	16.635	1.00	115.59	A
1816	O	SER	746	17.679	2.505	15.802	1.00	114.80	A
1817	N	ILE	747	19.668	1.807	16.627	1.00	114.95	A
1818	CA	ILE	747	20.531	2.397	15.609	1.00	113.53	A
1819	CB	ILE	747	21.545	3.387	16.244	1.00	113.48	A
1820	CG2	ILE	747	22.594	3.816	15.228	1.00	113.56	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1821	CG1	ILE	747	20.798	4.621	16.749	1.00	113.34	A
	1822	CD1	ILE	747	21.491	5.322	17.880	1.00	113.67	A
10	1823	C	ILE	747	21.238	1.158	15.051	1.00	112.59	A
	1824	O	ILE	747	21.829	0.380	15.803	1.00	112.41	A
	1825	N	GLU	748	21.146	0.974	13.738	1.00	111.41	A
15	1826	CA	GLU	748	21.718	-0.186	13.061	1.00	110.45	A
	1827	CB	GLU	748	20.920	-0.492	11.819	1.00	112.15	A
	1828	CG	GLU	748	19.542	-0.943	12.075	1.00	115.24	A
	1829	CD	GLU	748	18.913	-1.396	10.796	1.00	117.08	A
20	1830	OE1	GLU	748	19.522	-2.261	10.127	1.00	117.86	A
	1831	OE2	GLU	748	17.825	-0.885	10.456	1.00	118.10	A
	1832	C	GLU	748	23.161	-0.154	12.621	1.00	108.52	A
25	1833	O	GLU	748	23.593	0.773	11.946	1.00	108.69	A
	1834	N	PHE	749	23.891	-1.208	12.951	1.00	106.14	A
	1835	CA	PHE	749	25.277	-1.304	12.545	1.00	103.42	A
	1836	CB	PHE	749	26.137	-1.709	13.739	1.00	102.12	A
30	1837	CG	PHE	749	26.427	-0.574	14.688	1.00	100.46	A
	1838	CD1	PHE	749	25.485	-0.142	15.620	1.00	99.45	A
	1839	CD2	PHE	749	27.681	0.022	14.684	1.00	99.75	A
35	1840	CE1	PHE	749	25.793	0.876	16.522	1.00	98.95	A
	1841	CE2	PHE	749	27.999	1.034	15.576	1.00	99.15	A
	1842	CZ	PHE	749	27.061	1.449	16.506	1.00	98.78	A
40	1843	C	PHE	749	25.366	-2.336	11.424	1.00	102.03	A
	1844	O	PHE	749	24.849	-3.444	11.552	1.00	101.37	A
	1845	N	PRO	750	26.038	-1.998	10.306	1.00	101.19	A
	1846	CD	PRO	750	27.100	-0.995	10.107	1.00	101.23	A
45	1847	CA	PRO	750	26.090	-3.003	9.250	1.00	100.72	A
	1848	CB	PRO	750	26.774	-2.262	8.113	1.00	99.98	A
	1849	CG	PRO	750	27.812	-1.500	8.837	1.00	100.74	A
	1850	C	PRO	750	26.859	-4.235	9.708	1.00	100.57	A
50	1851	O	PRO	750	27.192	-4.365	10.885	1.00	100.03	A
	1852	N	GLU	751	27.145	-5.131	8.766	1.00	100.58	A
	1853	CA	GLU	751	27.847	-6.379	9.056	1.00	100.49	A
55	1854	CB	GLU	751	27.693	-7.331	7.875	1.00	101.63	A
	1855	CG	GLU	751	27.095	-8.689	8.227	1.00	103.13	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1856	CD	GLU	751	28.000	-9.557	9.106	1.00	105.13	A
1857	OE1	GLU	751	29.247	-9.505	8.971	1.00	106.54	A
1858	OE2	GLU	751	27.449	-10.321	9.922	1.00	104.89	A
1859	C	GLU	751	29.328	-6.227	9.382	1.00	99.40	A
1860	O	GLU	751	29.791	-6.650	10.444	1.00	98.23	A
1861	N	MET	752	30.074	-5.650	8.448	1.00	98.65	A
1862	CA	MET	752	31.494	-5.439	8.648	1.00	97.97	A
1863	CB	MET	752	32.015	-4.443	7.605	1.00	99.04	A
1864	CG	MET	752	33.487	-4.148	7.738	1.00	100.18	A
1865	SD	MET	752	34.387	-5.685	7.901	1.00	101.15	A
1866	CE	MET	752	34.323	-6.213	6.236	1.00	101.26	A
1867	C	MET	752	31.717	-4.907	10.066	1.00	96.84	A
1868	O	MET	752	32.232	-5.619	10.927	1.00	96.54	A
1869	N	LEU	753	31.299	-3.661	10.295	1.00	95.99	A
1870	CA	LEU	753	31.412	-2.979	11.591	1.00	94.98	A
1871	CB	LEU	753	30.655	-1.645	11.555	1.00	93.18	A
1872	CG	LEU	753	31.327	-0.282	11.406	1.00	91.40	A
1873	CD1	LEU	753	32.026	-0.142	10.073	1.00	90.81	A
1874	CD2	LEU	753	30.256	0.774	11.527	1.00	91.13	A
1875	C	LEU	753	30.841	-3.813	12.730	1.00	95.34	A
1876	O	LEU	753	31.353	-3.790	13.854	1.00	94.92	A
1877	N	ALA	754	29.756	-4.515	12.436	1.00	96.40	A
1878	CA	ALA	754	29.087	-5.365	13.413	1.00	97.52	A
1879	CB	ALA	754	28.056	-6.244	12.714	1.00	97.46	A
1880	C	ALA	754	30.127	-6.233	14.113	1.00	98.02	A
1881	O	ALA	754	30.257	-6.198	15.338	1.00	97.73	A
1882	N	GLU	755	30.864	-6.987	13.304	1.00	98.67	A
1883	CA	GLU	755	31.921	-7.905	13.742	1.00	99.35	A
1884	CB	GLU	755	32.477	-8.629	12.536	1.00	100.91	A
1885	CG	GLU	755	31.977	-10.010	12.322	1.00	103.15	A
1886	CD	GLU	755	32.582	-10.587	11.074	1.00	104.45	A
1887	OE1	GLU	755	33.424	-9.892	10.461	1.00	105.05	A
1888	OE2	GLU	755	32.222	-11.724	10.705	1.00	105.40	A
1889	C	GLU	755	33.116	-7.305	14.467	1.00	98.62	A
1890	O	GLU	755	33.579	-7.841	15.476	1.00	98.37	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1891	N	ILE	756	33.640	-6.227	13.892	1.00	97.94	A
	1892	CA	ILE	756	34.804	-5.512	14.401	1.00	97.06	A
10	1893	CB	ILE	756	35.249	-4.470	13.376	1.00	95.95	A
	1894	CG2	ILE	756	36.513	-3.783	13.830	1.00	95.40	A
	1895	CG1	ILE	756	35.484	-5.154	12.036	1.00	94.93	A
15	1896	CD1	ILE	756	35.420	-4.204	10.888	1.00	95.21	A
	1897	C	ILE	756	34.544	-4.832	15.740	1.00	97.25	A
	1898	O	ILE	756	35.461	-4.693	16.556	1.00	97.09	A
	1899	N	ILE	757	33.304	-4.387	15.960	1.00	97.46	A
20	1900	CA	ILE	757	32.953	-3.754	17.227	1.00	98.19	A
	1901	CB	ILE	757	31.636	-2.904	17.129	1.00	97.65	A
	1902	CG2	ILE	757	31.194	-2.467	18.522	1.00	97.21	A
25	1903	CG1	ILE	757	31.890	-1.625	16.312	1.00	97.77	A
	1904	CD1	ILE	757	30.718	-1.146	15.454	1.00	97.25	A
	1905	C	ILE	757	32.805	-4.872	18.265	1.00	99.15	A
	1906	O	ILE	757	33.306	-4.746	19.382	1.00	99.19	A
30	1907	N	THR	758	32.141	-5.968	17.884	1.00	100.27	A
	1908	CA	THR	758	31.964	-7.130	18.768	1.00	101.43	A
	1909	CB	THR	758	31.082	-8.230	18.101	1.00	101.61	A
35	1910	OG1	THR	758	31.053	-8.021	16.686	1.00	101.89	A
	1911	CG2	THR	758	29.660	-8.206	18.650	1.00	101.75	A
	1912	C	THR	758	33.339	-7.733	19.066	1.00	102.09	A
	1913	O	THR	758	33.629	-8.149	20.188	1.00	101.89	A
40	1914	N	ASN	759	34.175	-7.774	18.035	1.00	103.34	A
	1915	CA	ASN	759	35.540	-8.289	18.108	1.00	105.16	A
	1916	CB	ASN	759	36.231	-8.027	16.760	1.00	105.72	A
45	1917	CG	ASN	759	37.652	-8.573	16.687	1.00	106.18	A
	1918	OD1	ASN	759	38.488	-8.313	17.556	1.00	105.89	A
	1919	ND2	ASN	759	37.934	-9.320	15.625	1.00	106.34	A
	1920	C	ASN	759	36.288	-7.557	19.223	1.00	106.31	A
50	1921	O	ASN	759	36.597	-8.120	20.273	1.00	106.83	A
	1922	N	GLN	760	36.542	-6.283	18.957	1.00	107.80	A
	1923	CA	GLN	760	37.273	-5.351	19.815	1.00	109.24	A
55	1924	CB	GLN	760	37.375	-4.032	19.067	1.00	109.55	A
	1925	CG	GLN	760	38.163	-4.174	17.815	1.00	110.53	A

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1926	CD	GLN	760	39.548	-4.664	18.132	1.00	111.49	A
1927	OE1	GLN	760	39.918	-5.791	17.804	1.00	111.90	A
1928	NE2	GLN	760	40.323	-3.823	18.806	1.00	112.26	A
1929	C	GLN	760	36.782	-5.052	21.223	1.00	109.82	A
1930	O	GLN	760	37.575	-4.916	22.161	1.00	108.95	A
1931	N	ILE	761	35.468	-4.924	21.334	1.00	111.38	A
1932	CA	ILE	761	34.793	-4.577	22.573	1.00	113.13	A
1933	CB	ILE	761	33.247	-4.839	22.414	1.00	112.25	A
1934	CG2	ILE	761	32.949	-6.322	22.323	1.00	112.15	A
1935	CG1	ILE	761	32.470	-4.200	23.561	1.00	111.65	A
1936	CD1	ILE	761	32.594	-4.922	24.877	1.00	111.27	A
1937	C	ILE	761	35.364	-5.187	23.862	1.00	114.87	A
1938	O	ILE	761	35.448	-4.502	24.885	1.00	115.06	A
1939	N	PRO	762	35.787	-6.461	23.834	1.00	116.56	A
1940	CD	PRO	762	35.597	-7.519	22.831	1.00	116.88	A
1941	CA	PRO	762	36.330	-7.031	25.069	1.00	117.98	A
1942	CB	PRO	762	36.454	-8.516	24.737	1.00	117.53	A
1943	CG	PRO	762	35.390	-8.723	23.703	1.00	117.09	A
1944	C	PRO	762	37.671	-6.424	25.465	1.00	119.34	A
1945	O	PRO	762	37.813	-5.854	26.545	1.00	119.13	A
1946	N	LYS	763	38.649	-6.529	24.571	1.00	121.52	A
1947	CA	LYS	763	39.988	-6.025	24.853	1.00	123.89	A
1948	CB	LYS	763	41.025	-6.777	24.007	1.00	124.50	A
1949	CG	LYS	763	41.377	-6.076	22.701	1.00	125.11	A
1950	CD	LYS	763	40.640	-6.658	21.513	1.00	125.37	A
1951	CE	LYS	763	41.386	-7.881	21.002	1.00	126.09	A
1952	NZ	LYS	763	40.789	-8.514	19.792	1.00	126.47	A
1953	C	LYS	763	40.250	-4.519	24.709	1.00	125.24	A
1954	O	LYS	763	41.364	-4.077	24.995	1.00	125.51	A
1955	N	TYR	764	39.271	-3.728	24.259	1.00	126.66	A
1956	CA	TYR	764	39.504	-2.280	24.123	1.00	127.39	A
1957	CB	TYR	764	38.628	-1.648	23.025	1.00	128.05	A
1958	CG	TYR	764	39.451	-0.985	21.937	1.00	129.02	A
1959	CD1	TYR	764	39.575	-1.577	20.681	1.00	129.21	A
1960	CE1	TYR	764	40.445	-1.064	19.718	1.00	129.52	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	1961	CD2	TYR	764	40.206	0.163	22.203	1.00	129.22	A
	1962	CE2	TYR	764	41.085	0.687	21.243	1.00	129.70	A
10	1963	CZ	TYR	764	41.203	0.061	20.006	1.00	129.81	A
	1964	OH	TYR	764	42.124	0.504	19.083	1.00	129.43	A
	1965	C	TYR	764	39.221	-1.570	25.434	1.00	127.40	A
15	1966	O	TYR	764	38.978	-0.365	25.451	1.00	127.67	A
	1967	N	SER	765	39.274	-2.330	26.525	1.00	127.42	A
	1968	CA	SER	765	38.999	-1.807	27.858	1.00	127.37	A
	1969	CB	SER	765	37.552	-2.121	28.245	1.00	127.92	A
20	1970	OG	SER	765	36.660	-1.906	27.166	1.00	128.95	A
	1971	C	SER	765	39.908	-2.405	28.928	1.00	126.95	A
	1972	O	SER	765	40.246	-1.738	29.908	1.00	127.13	A
25	1973	N	ASN	766	40.290	-3.668	28.735	1.00	126.33	A
	1974	CA	ASN	766	41.121	-4.420	29.682	1.00	125.68	A
	1975	CB	ASN	766	41.166	-5.899	29.271	1.00	126.48	A
	1976	CG	ASN	766	39.788	-6.497	29.051	1.00	127.50	A
30	1977	OD1	ASN	766	38.850	-6.221	29.803	1.00	128.09	A
	1978	ND2	ASN	766	39.660	-7.339	28.026	1.00	127.55	A
	1979	C	ASN	766	42.559	-3.958	29.915	1.00	124.54	A
35	1980	O	ASN	766	42.970	-3.691	31.052	1.00	124.51	A
	1981	N	GLY	767	43.324	-3.891	28.833	1.00	122.93	A
	1982	CA	GLY	767	44.722	-3.509	28.903	1.00	120.80	A
40	1983	C	GLY	767	45.416	-4.524	28.018	1.00	119.01	A
	1984	O	GLY	767	46.310	-5.259	28.440	1.00	118.79	A
	1985	N	ASN	768	44.973	-4.564	26.773	1.00	117.24	A
	1986	CA	ASN	768	45.504	-5.506	25.810	1.00	115.20	A
45	1987	CB	ASN	768	44.318	-6.304	25.223	1.00	116.68	A
	1988	CG	ASN	768	43.414	-6.926	26.320	1.00	118.09	A
	1989	OD1	ASN	768	43.106	-6.281	27.331	1.00	118.30	A
50	1990	ND2	ASN	768	42.984	-8.171	26.105	1.00	118.06	A
	1991	C	ASN	768	46.307	-4.776	24.718	1.00	113.01	A
	1992	O	ASN	768	47.374	-5.237	24.309	1.00	112.58	A
	1993	N	ILE	769	45.805	-3.608	24.305	1.00	109.95	A
55	1994	CA	ILE	769	46.388	-2.762	23.252	1.00	106.52	A
	1995	CB	ILE	769	45.260	-1.996	22.527	1.00	106.78	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1996	CG2	ILE	769	45.826	-1.167	21.379	1.00	106.69	A
1997	CG1	ILE	769	44.197	-2.994	22.053	1.00	106.81	A
1998	CD1	ILE	769	42.973	-2.369	21.435	1.00	106.29	A
1999	C	ILE	769	47.463	-1.732	23.664	1.00	103.81	A
2000	O	ILE	769	47.264	-0.935	24.582	1.00	103.59	A
2001	N	LYS	770	48.585	-1.735	22.947	1.00	100.30	A
2002	CA	LYS	770	49.691	-0.824	23.218	1.00	96.45	A
2003	CB	LYS	770	51.001	-1.579	23.072	1.00	95.81	A
2004	CG	LYS	770	52.227	-0.777	23.354	1.00	94.18	A
2005	CD	LYS	770	53.407	-1.532	22.808	1.00	94.37	A
2006	CE	LYS	770	54.692	-0.768	23.017	1.00	93.82	A
2007	NZ	LYS	770	55.821	-1.401	22.284	1.00	93.42	A
2008	C	LYS	770	49.676	0.360	22.250	1.00	94.29	A
2009	O	LYS	770	50.038	0.228	21.082	1.00	94.06	A
2010	N	LYS	771	49.272	1.517	22.756	1.00	91.57	A
2011 1	CA	LYS	771	49.174	2.727	21.949	1.00	88.83	A
2012	CB	LYS	771	48.176	3.678	22.654	1.00	88.60	A
2013	CG	LYS	771	46.931	2.902	23.212	1.00	89.92	A
2014	CD	LYS	771	45.687	3.749	23.550	1.00	90.42	A
2015	CE	LYS	771	45.830	4.541	24.848	1.00	92.04	A
2016	NZ	LYS	771	45.010	5.799	24.853	1.00	92.59	A
2017	C	LYS	771	50.547	3.392	21.692	1.00	86.56	A
2018	O	LYS	771	51.009	4.180	22.506	1.00	86.88	A
2019	N	LEU	772	51.200	3.067	20.571	1.00	83.82	A
2020	CA	LEU	772	52.510	3.650	20.229	1.00	81.98	A
2021	CB	LEU	772	52.970	3.194	18.838	1.00	80.07	A
2022	CG	LEU	772	52.856	1.704	18.545	1.00	78.83	A
2023	CD1	LEU	772	53.382	1.346	17.159	1.00	78.33	A
2024	CD2	LEU	772	53.635	0.984	19.605	1.00	78.33	A
2025	C	LEU	772	52.424	5.176	20.219	1.00	82.19	A
2026	O	LEU	772	51.397	5.735	19.839	1.00	82.51	A
2027	N	LEU	773	53.492	5.857	20.620	1.00	81.85	A
2028	CA	LEU	773	53.476	7.320	20.617	1.00	81.81	A
2029	CB	LEU	773	53.261	7.871	22.027	1.00	80.64	A
2030	CG	LEU	773	51.990	7.525	22.798	1.00	79.78	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2031	CD1	LEU	773	52.296	7.672	24.267	1.00	80.42	A
	2032	CD2	LEU	773	50.826	8.418	22.396	1.00	79.59	A
10	2033	C	LEU	773	54.786	7.878	20.082	1.00	82.31	A
	2034	O	LEU	773	55.849	7.320	20.341	1.00	82.88	A
	2035	N	PHE	774	54.705	8.972	19.331	1.00	82.39	A
15	2036	CA	PHE	774	55.895	9.612	18.798	1.00	82.78	A
	2037	CB	PHE	774	55.538	10.531	17.630	1.00	80.87	A
	2038	CG	PHE	774	55.321	9.799	16.353	1.00	78.91	A
	2039	CD1	PHE	774	56.395	9.479	15.539	1.00	78.24	A
20	2040	CD2	PHE	774	54.064	9.292	16.038	1.00	78.78	A
	2041	CE1	PHE	774	56.226	8.654	14.428	1.00	78.15	A
	2042	CE2	PHE	774	53.881	8.465	14.931	1.00	78.23	A
25	2043	CZ	PHE	774	54.966	8.143	14.127	1.00	78.32	A
	2044	C	PHE	774	56.498	10.406	19.933	1.00	84.83	A
	2045	O	PHE	774	57.704	10.639	19.968	1.00	84.81	A
	2046	N	HIS	775	55.638	10.796	20.873	1.00	88.32	A
30	2047	CA	HIS	775	56.039	11.578	22.041	1.00	91.73	A
	2048	CB	HIS	775	55.558	13.012	21.895	1.00	90.90	A
	2049	CG	HIS	775	55.970	13.634	20.612	1.00	90.80	A
35	2050	CD2	HIS	775	55.263	14.275	19.656	1.00	90.67	A
	2051	ND1	HIS	775	57.265	13.551	20.143	1.00	90.62	A
	2052	CE1	HIS	775	57.333	14.107	18.950	1.00	91.01	A
	2053	NE2	HIS	775	56.131	14.554	18.629	1.00	91.35	A
40	2054	C	HIS	775	55.506	11.026	23.340	1.00	94.76	A
	2055	O	HIS	775	54.304	10.790	23.480	1.00	94.90	A
	2056	N	GLN	776	56.398	10.841	24.303	1.00	98.84	A
45	2057	CA	GLN	776	55.996	10.334	25.601	1.00	103.31	A
	2058	CB	GLN	776	57.179	9.633	26.291	1.00	104.45	A
	2059	CG	GLN	776	58.582	10.114	25.886	1.00	106.57	A
	2060	CD	GLN	776	58.999	11.424	26.551	1.00	108.35	A
50	2061	OE1	GLN	776	58.837	12.508	25.981	1.00	108.79	A
	2062	NE2	GLN	776	59.538	11.323	27.767	1.00	108.32	A
	2063	C	GLN	776	55.384	11.412	26.511	1.00	105.64	A
55	2064	O	GLN	776	54.217	11.295	26.883	1.00	106.06	A
	2065	N	LYS	777	56.149	12.466	26.822	1.00	108.50	A

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2066	CA	LYS	777	55.725	13.569	27.721	1.00	111.14	A
2067	CB	LYS	777	55.127	14.778	26.940	1.00	111.13	A
2068	CG	LYS	777	55.167	16.163	27.704	1.00	111.26	A
2069	CD	LYS	777	53.761	16.804	27.916	1.00	110.94	A
2070	CE	LYS	777	53.775	18.216	28.568	1.00	110.88	A
2071	NZ	LYS	777	54.016	18.255	30.049	1.00	110.23	A
2072	C	LYS	777	54.728	13.077	28.778	1.00	112.33	A
2073	O	LYS	777	53.497	13.179	28.558	1.00	112.91	A
2074	OXT	LYS	777	55.202	12.561	29.818	1.00	113.31	A
2075	CB	LYS	740	36.212	-17.177	16.526	1.00	126.78	B
2076	CG	LYS	740	36.506	-17.638	17.979	1.00	128.08	B
2077	CD	LYS	740	37.327	-18.909	18.063	1.00	129.35	B
2078	CE	LYS	740	38.818	-18.624	18.192	1.00	129.72	B
2079	NZ	LYS	740	39.630	-19.761	17.686	1.00	130.22	B
2080	C	LYS	740	37.246	-15.433	15.072	1.00	124.52	B
2081	O	LYS	740	37.988	-14.994	14.192	1.00	124.88	B
2082	N	LYS	740	38.637	-16.592	16.502	1.00	126.10	B
2083	CA	LYS	740	37.432	-16.814	15.655	1.00	125.59	B
2084	N	GLU	741	36.239	-14.769	15.618	1.00	122.85	B
2085	CA	GLU	741	35.871	-13.404	15.324	1.00	120.66	B
2086	CB	GLU	741	36.304	-12.556	16.511	1.00	121.44	B
2087	CG	GLU	741	35.820	-13.120	17.844	1.00	121.77	B
2088	CD	GLU	741	36.524	-14.406	18.271	1.00	122.23	B
2089	OE1	GLU	741	37.767	-14.406	18.439	1.00	122.26	B
2090	OE2	GLU	741	35.811	-15.408	18.452	1.00	121.76	B
2091	C	GLU	741	36.317	-12.740	14.032	1.00	118.57	B
2092	O	GLU	741	37.480	-12.798	13.620	1.00	118.23	B
2093	N	ASN	742	35.345	-12.103	13.398	1.00	116.10	B
2094	CA	ASN	742	35.600	-11.375	12.184	1.00	113.26	B
2095	CB	ASN	742	36.529	-10.220	12.514	1.00	114.33	B
2096	CG	ASN	742	36.603	-9.208	11.418	1.00	115.13	B
2097	OD1	ASN	742	37.244	-8.171	11.572	1.00	116.52	B
2098	ND2	ASN	742	35.948	-9.494	10.297	1.00	114.81	B
2099	C	ASN	742	36.204	-12.247	11.094	1.00	110.51	B
2100	O	ASN	742	37.313	-11.999	10.623	1.00	110.08	B

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2101	N	ALA	743	35.473	-13.285	10.702	1.00	106.82	B
	2102	CA	ALA	743	35.952	-14.143	9.640	1.00	102.91	B
10	2103	CB	ALA	743	35.161	-15.450	9.610	1.00	103.22	B
	2104	C	ALA	743	35.745	-13.344	8.355	1.00	100.03	B
	2105	O	ALA	743	36.397	-13.611	7.345	1.00	99.90	B
15	2106	N	LEU	744	34.861	-12.344	8.400	1.00	95.91	B
	2107	CA	LEU	744	34.588	-11.513	7.224	1.00	92.30	B
	2108	CB	LEU	744	33.374	-10.603	7.455	1.00	91.74	B
	2109	CG	LEU	744	32.438	-10.333	6.259	1.00	91.66	B
20	2110	CD1	LEU	744	31.463	-9.223	6.623	1.00	91.11	B
	2111	CD2	LEU	744	33.221	-9.924	5.023	1.00	92.05	B
	2112	C	LEU	744	35.793	-10.662	6.779	1.00	90.60	B
25	2113	O	LEU	744	35.905	-10.346	5.596	1.00	90.25	B
	2114	N	LEU	745	36.680	-10.274	7.695	1.00	87.95	B
	2115	CA	LEU	745	37.872	-9.492	7.312	1.00	85.36	B
	2116	CB	LEU	745	38.474	-8.746	8.502	1.00	84.07	B
30	2117	CG	LEU	745	38.669	-7.237	8.665	1.00	82.29	B
	2118	CD1	LEU	745	39.514	-7.118	9.916	1.00	80.83	B
	2119	CD2	LEU	745	39.362	-6.537	7.497	1.00	80.58	B
35	2120	C	LEU	745	38.921	-10.486	6.839	1.00	84.43	B
	2121	O	LEU	745	39.672	-10.226	5.894	1.00	84.16	B
	2122	N	ARG	746	38.987	-11.616	7.541	1.00	83.85	B
	2123	CA	ARG	746	39.926	-12.673	7.209	1.00	83.05	B
40	2124	CB	ARG	746	39.707	-13.898	8.097	1.00	83.28	B
	2125	CG	ARG	746	40.511	-15.126	7.673	1.00	84.87	B
	2126	CD	ARG	746	40.606	-16.167	8.792	1.00	86.65	B
45	2127	NE	ARG	746	41.854	-16.040	9.554	1.00	89.65	B
	2128	CZ	ARG	746	41.934	-15.874	10.874	1.00	90.19	B
	2129	NH1	ARG	746	40.829	-15.809	11.618	1.00	90.02	B
	2130	NH2	ARG	746	43.128	-15.766	11.455	1.00	88.90	B
50	2131	C	ARG	746	39.689	-13.043	5.768	1.00	82.22	B
	2132	O	ARG	746	40.614	-13.204	4.998	1.00	82.49	B
	2133	N	TYR	747	38.428	-13.155	5.409	1.00	82.19	B
55	2134	CA	TYR	747	38.059	-13.508	4.058	1.00	82.92	B
	2135	CB	TYR	747	36.555	-13.717	4.010	1.00	82.63	B

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2136	CG	TYR	747	36.065	-13.789	2.616	1.00	82.87	B
2137	CD1	TYR	747	36.594	-14.724	1.734	1.00	83.81	B
2138	CE1	TYR	747	36.209	-14.756	0.422	1.00	84.67	B
2139	CD2	TYR	747	35.130	-12.884	2.147	1.00	82.83	B
2140	CE2	TYR	747	34.732	-12.903	0.833	1.00	84.05	B
2141	CZ	TYR	747	35.276	-13.840	-0.026	1.00	85.10	B
2142	OH	TYR	747	34.880	-13.863	-1.336	1.00	86.88	B
2143	C	TYR	747	38.479	-12.448	3.022	1.00	83.86	B
2144	O	TYR	747	38.943	-12.768	1.917	1.00	84.05	B
2145	N	LEU	748	38.296	-11.189	3.414	1.00	84.91	B
2146	CA	LEU	748	38.593	-9.994	2.622	1.00	85.00	B
2147	CB	LEU	748	38.142	-8.763	3.391	1.00	85.05	B
2148	CG	LEU	748	36.733	-8.194	3.274	1.00	84.64	B
2149	CD1	LEU	748	36.515	-7.239	4.426	1.00	85.29	B
2150	CD2	LEU	748	36.573	-7.473	1.947	1.00	83.89	B
2151	C	LEU	748	40.063	-9.807	2.299	1.00	85.69	B
2152	O	LEU	748	40.429	-9.385	1.197	1.00	85.46	B
2153	N	LEU	749	40.886	-10.089	3.294	1.00	87.36	B
2154	CA	LEU	749	42.329	-9.958	3.191	1.00	90.50	B
2155	CB	LEU	749	42.948	-10.171	4.574	1.00	87.67	B
2156	CG	LEU	749	42.539	-9.094	5.578	1.00	85.91	B
2157	CD1	LEU	749	43.126	-9.325	6.963	1.00	84.27	B
2158	CD2	LEU	749	43.012	-7.775	5.016	1.00	83.58	B
2159	C	LEU	749	42.971	-10.913	2.199	1.00	94.62	B
2160	O	LEU	749	44.057	-10.645	1.683	1.00	95.29	B
2161	N	ASP	750	42.293	-12.010	1.906	1.00	99.41	B
2162	CA	ASP	750	42.859	-13.007	1.025	1.00	103.90	B
2163	CB	ASP	750	42.303	-14.362	1.502	1.00	103.66	B
2164	CG	ASP	750	42.735	-14.686	2.957	1.00	103.87	B
2165	OD1	ASP	750	43.483	-15.661	3.178	1.00	103.14	B
2166	OD2	ASP	750	42.347	-13.947	3.885	1.00	104.73	B
2167	C	ASP	750	42.856	-12.811	-0.534	1.00	108.04	B
2168	O	ASP	750	43.917	-12.898	-1.140	1.00	108.70	B
2169	N	LYS	751	41.728	-12.458	-1.161	1.00	112.20	B
2170	CA	LYS	751	41.571	-12.287	-2.648	1.00	117.11	B

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2171	CB	LYS	751	40.158	-12.770	-2.987	1.00	117.68	B
	2172	CG	LYS	751	39.095	-12.327	-1.933	1.00	118.08	B
10	2173	CD	LYS	751	39.319	-10.912	-1.354	1.00	118.35	B
	2174	CE	LYS	751	38.613	-9.832	-2.158	1.00	118.66	B
	2175	NZ	LYS	751	37.151	-10.073	-2.164	1.00	118.89	B
15	2176	C	LYS	751	41.736	-10.959	-3.494	1.00	120.57	B
	2177	O	LYS	751	40.815	-10.163	-3.467	1.00	120.77	B
	2178	N	ASP	752	42.787	-10.662	-4.272	1.00	124.55	B
	2179	CA	ASP	752	42.641	-9.379	-5.042	1.00	128.27	B
20	2180	CB	ASP	752	43.242	-8.168	-4.270	1.00	128.97	B
	2181	CG	ASP	752	42.370	-6.877	-4.391	1.00	130.06	B
	2182	OD1	ASP	752	42.081	-6.432	-5.529	1.00	130.65	B
25	2183	OD2	ASP	752	41.975	-6.299	-3.348	1.00	130.15	B
	2184	C	ASP	752	43.041	-9.284	-6.550	1.00	129.74	B
	2185	O	ASP	752	42.531	-8.403	-7.257	1.00	130.16	B
	2186	N	ASP	753	43.903	-10.186	-7.031	1.00	131.88	B
30	2187	CA	ASP	753	44.382	-10.237	-8.438	1.00	132.79	B
	2188	CB	ASP	753	44.786	-11.700	-8.767	1.00	133.26	B
	2189	CG	ASP	753	45.584	-11.841	-10.074	1.00	133.42	B
35	2190	OD1	ASP	753	44.982	-11.747	-11.168	1.00	133.48	B
	2191	OD2	ASP	753	46.815	-12.067	-10.003	1.00	133.16	B
	2192	C	ASP	753	43.364	-9.707	-9.474	1.00	133.27	B
	2193	O	ASP	753	43.309	-8.468	-9.660	1.00	133.47	B
40	2194	OXT	ASP	753	42.624	-10.518	-10.079	1.00	133.68	B
	2195	CB	LEU	525	40.004	46.082	16.396	1.00	136.92	D
	2196	CG	LEU	525	39.293	45.409	15.212	1.00	137.30	D
45	2197	CD1	LEU	525	39.125	46.375	14.046	1.00	136.87	D
	2198	CD2	LEU	525	40.098	44.179	14.790	1.00	137.28	D
	2199	C	LEU	525	37.974	47.434	17.108	1.00	135.85	D
	2200	O	LEU	525	37.316	46.395	17.075	1.00	136.26	D
50	2201	N	LEU	525	40.125	47.532	18.398	1.00	136.62	D
	2202	CA	LEU	525	39.512	47.393	17.042	1.00	136.44	D
	2203	N	PRO	526	37.390	48.641	17.246	1.00	134.93	D
55	2204	CD	PRO	526	38.029	49.714	18.037	1.00	134.90	D
	2205	CA	PRO	526	35.929	48.780	17.315	1.00	133.52	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2206	CB	PRO	526	35.730	49.375	18.690	1.00	134.35	D
2207	CG	PRO	526	36.830	50.415	18.709	1.00	134.90	D
2208	C	PRO	526	35.316	49.692	16.243	1.00	131.67	D
2209	O	PRO	526	35.089	50.875	16.504	1.00	131.68	D
2210	N	GLN	527	35.017	49.166	15.064	1.00	129.15	D
2211	CA	GLN	527	34.438	50.023	14.038	1.00	126.46	D
2212	CB	GLN	527	34.671	49.401	12.657	1.00	126.52	D
2213	CG	GLN	527	34.626	47.894	12.636	1.00	126.83	D
2214	CD	GLN	527	33.233	47.385	12.865	1.00	127.18	D
2215	OE1	GLN	527	32.264	48.096	12.616	1.00	126.89	D
2216	NE2	GLN	527	32.264	48.096	12.616	1.00	128.15	D
2217	C	GLN	527	33.117	46.143	13.324	1.00	124.32	D
2218	O	GLN	527	32.955	50.431	14.241	1.00	124.28	D
2219	N	LEU	528	32.591	51.569	13.921	1.00	121.31	D
2220	CA	LEU	528	32.128	49.533	14.798	1.00	121.31	D
2221	CB	LEU	528	30.684	49.773	15.072	1.00	117.75	D
2222	CG	LEU	528	30.468	50.286	16.503	1.00	118.19	D
2223	CD1	LEU	528	30.468	50.286	16.503	1.00	118.67	D
2224	CD2	LEU	528	30.502	49.369	17.727	1.00	118.31	D
2225	C	LEU	528	31.761	48.525	17.715	1.00	118.31	D
2226	O	LEU	528	30.435	50.226	18.991	1.00	119.12	D
2227	N	THR	529	30.435	50.226	18.991	1.00	114.85	D
2228	CA	THR	529	29.995	50.749	14.125	1.00	114.46	D
2229	CB	THR	529	29.206	51.591	14.558	1.00	114.46	D
2230	OG1	THR	529	29.206	51.591	14.558	1.00	111.72	D
2231	CG2	THR	529	30.275	50.614	12.840	1.00	111.72	D
2232	C	THR	529	30.275	50.614	12.840	1.00	107.57	D
2233	O	THR	529	29.727	51.501	11.831	1.00	107.57	D
2234	N	PRO	530	29.727	51.501	11.831	1.00	107.58	D
2235	CD	PRO	530	30.647	52.757	11.723	1.00	107.58	D
2236	CA	PRO	530	30.647	52.757	11.723	1.00	108.51	D
2237	CB	PRO	530	29.965	53.809	11.038	1.00	108.51	D
2238	CG	PRO	530	29.965	53.809	11.038	1.00	106.76	D
2239	C	PRO	530	29.965	53.809	11.038	1.00	106.76	D
2240	O	PRO	530	31.949	52.426	11.009	1.00	106.76	D
				29.655	50.697	10.519	1.00	104.56	D
				30.679	50.281	9.969	1.00	104.85	D
				28.434	50.463	10.012	1.00	100.85	D
				27.221	51.206	10.399	1.00	100.11	D
				28.190	49.697	8.785	1.00	97.13	D
				26.672	49.710	8.679	1.00	98.21	D
				26.344	51.081	9.162	1.00	98.89	D
				28.842	50.242	7.531	1.00	93.39	D
				28.791	51.438	7.261	1.00	92.57	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2241	N	THR	531	29.470	49.353	6.775	1.00	89.92	D
	2242	CA	THR	531	30.077	49.750	5.522	1.00	86.89	D
10	2243	CB	THR	531	31.470	49.126	5.304	1.00	86.90	D
	2244	OG1	THR	531	31.412	47.706	5.492	1.00	86.36	D
	2245	CG2	THR	531	32.469	49.726	6.266	1.00	86.26	D
15	2246	C	THR	531	29.102	49.196	4.519	1.00	85.27	D
	2247	O	THR	531	28.306	48.316	4.846	1.00	85.29	D
	2248	N	LEU	532	29.142	49.701	3.301	1.00	82.89	D
	2249	CA	LEU	532	28.206	49.223	2.306	1.00	80.97	D
20	2250	CB	LEU	532	28.380	50.042	1.047	1.00	79.96	D
	2251	CG	LEU	532	27.321	49.899	-0.032	1.00	79.61	D
	2252	CD1	LEU	532	25.947	49.459	0.495	1.00	79.10	D
25	2253	CD2	LEU	532	27.255	51.256	-0.674	1.00	79.67	D
	2254	C	LEU	532	28.357	47.725	2.018	1.00	80.18	D
	2255	O	LEU	532	27.367	47.000	1.884	1.00	80.38	D
	2256	N	VAL	533	29.597	47.261	1.925	1.00	78.45	D
30	2257	CA	VAL	533	29.858	45.854	1.672	1.00	76.93	D
	2258	CB	VAL	533	31.319	45.637	1.290	1.00	75.90	D
	2259	CG1	VAL	533	32.198	46.022	2.461	1.00	75.17	D
35	2260	CG2	VAL	533	31.556	44.189	0.891	1.00	75.29	D
	2261	C	VAL	533	29.583	45.085	2.964	1.00	76.53	D
	2262	O	VAL	533	29.442	43.862	2.963	1.00	76.16	D
	2263	N	SER	534	29.520	45.818	4.073	1.00	75.87	D
40	2264	CA	SER	534	29.273	45.220	5.383	1.00	75.27	D
	2265	CB	SER	534	29.453	46.268	6.473	1.00	76.08	D
	2266	OG	SER	534	29.059	45.758	7.732	1.00	78.01	D
45	2267	C	SER	534	27.856	44.695	5.459	1.00	74.06	D
	2268	O	SER	534	27.574	43.601	5.941	1.00	73.87	D
	2269	N	LEU	535	26.963	45.531	4.978	1.00	73.15	D
	2270	CA	LEU	535	25.563	45.243	4.961	1.00	72.35	D
50	2271	CB	LEU	535	24.859	46.543	4.681	1.00	71.21	D
	2272	CG	LEU	535	23.382	46.585	4.898	1.00	69.96	D
	2273	CD1	LEU	535	23.089	47.679	5.872	1.00	70.31	D
55	2274	CD2	LEU	535	22.712	46.857	3.603	1.00	69.87	D
	2275	C	LEU	535	25.298	44.234	3.861	1.00	72.57	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2276	O	LEU	535	24.392	43.407	3.954	1.00	73.83	D
2277	N	LEU	536	26.099	44.301	2.807	1.00	72.53	D
2278	CA	LEU	536	25.931	43.381	1.694	1.00	72.36	D
2279	CB	LEU	536	26.849	43.814	0.551	1.00	71.10	D
2280	CG	LEU	536	26.370	43.781	-0.901	1.00	69.77	D
2281	CD1	LEU	536	25.018	44.439	-1.100	1.00	69.03	D
2282	CD2	LEU	536	27.415	44.504	-1.704	1.00	70.87	D
2283	C	LEU	536	26.256	41.957	2.180	1.00	72.62	D
2284	O	LEU	536	25.642	40.979	1.755	1.00	71.52	D
2285	N	GLU	537	27.210	41.845	3.092	1.00	73.92	D
2286	CA	GLU	537	27.545	40.540	3.608	1.00	74.65	D
2287	CB	GLU	537	28.921	40.555	4.242	1.00	75.29	D
2288	CG	GLU	537	29.255	39.278	4.954	1.00	78.75	D
2289	CD	GLU	537	30.683	39.277	5.451	1.00	81.31	D
2290	OE1	GLU	537	31.079	38.285	6.108	1.00	82.53	D
2291	OE2	GLU	537	31.407	40.268	5.177	1.00	80.17	D
2292	C	GLU	537	26.515	40.027	4.614	1.00	74.98	D
2293	O	GLU	537	26.170	38.852	4.566	1.00	76.28	D
2294	N	VAL	538	26.001	40.870	5.515	1.00	74.17	D
2295	CA	VAL	538	25.034	40.334	6.481	1.00	72.78	D
2296	CB	VAL	538	24.761	41.266	7.717	1.00	72.66	D
2297	CG1	VAL	538	26.006	42.046	8.094	1.00	72.43	D
2298	CG2	VAL	538	23.564	42.173	7.459	1.00	72.20	D
2299	C	VAL	538	23.680	39.951	5.898	1.00	72.50	D
2300	O	VAL	538	22.906	39.274	6.572	1.00	72.58	D
2301	N	ILE	539	23.375	40.364	4.666	1.00	71.88	D
2302	CA	ILE	539	22.085	40.005	4.067	1.00	71.03	D
2303	CB	ILE	539	21.374	41.207	3.399	1.00	70.22	D
2304	CG2	ILE	539	21.461	42.433	4.285	1.00	70.64	D
2305	CG1	ILE	539	21.997	41.492	2.033	1.00	69.87	D
2306	CD1	ILE	539	21.296	42.585	1.269	1.00	68.95	D
2307	C	ILE	539	22.209	38.920	3.006	1.00	71.27	D
2308	O	ILE	539	21.273	38.684	2.240	1.00	71.30	D
2309	N	GLU	540	23.365	38.269	2.954	1.00	71.95	D
2310	CA	GLU	540	23.598	37.216	1.980	1.00	73.04	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2311	CB	GLU	540	25.062	36.776	2.025	1.00	73.24	D
	2312	CG	GLU	540	25.494	35.779	0.948	1.00	75.23	D
10	2313	CD	GLU	540	24.963	36.111	-0.445	1.00	77.05	D
	2314	OE1	GLU	540	24.820	37.315	-0.762	1.00	77.82	D
	2315	OE2	GLU	540	24.703	35.165	-1.225	1.00	76.49	D
15	2316	C	GLU	540	22.692	36.060	2.337	1.00	73.74	D
	2317	O	GLU	540	22.561	35.719	3.505	1.00	74.01	D
	2318	N	PRO	541	21.993	35.496	1.355	1.00	75.38	D
	2319	CD	PRO	541	21.359	36.155	0.205	1.00	75.60	D
20	2320	CA	PRO	541	21.174	34.389	1.854	1.00	77.84	D
	2321	CB	PRO	541	20.270	34.029	0.671	1.00	77.22	D
	2322	CG	PRO	541	20.590	35.041	-0.424	1.00	76.96	D
25	2323	C	PRO	541	22.058	33.228	2.297	1.00	80.33	D
	2324	O	PRO	541	23.264	33.203	2.028	1.00	80.53	D
	2325	N	GLU	542	21.472	32.270	2.992	1.00	83.14	D
	2326	CA	GLU	542	22.262	31.149	3.446	1.00	86.12	D
30	2327	CB	GLU	542	21.979	30.892	4.904	1.00	88.33	D
	2328	CG	GLU	542	20.557	30.563	5.158	1.00	92.41	D
	2329	CD	GLU	542	20.435	29.825	6.445	1.00	96.11	D
35	2330	OE1	GLU	542	21.234	30.135	7.359	1.00	97.98	D
	2331	OE2	GLU	542	19.555	28.944	6.546	1.00	97.94	D
	2332	C	GLU	542	21.913	29.929	2.617	1.00	86.19	D
	2333	O	GLU	542	20.767	29.780	2.193	1.00	86.63	D
40	2334	N	VAL	543	22.895	29.060	2.388	1.00	86.32	D
	2335	CA	VAL	543	22.674	27.871	1.570	1.00	86.78	D
	2336	CB	VAL	543	23.891	26.926	1.557	1.00	87.17	D
45	2337	CG1	VAL	543	25.039	27.566	0.808	1.00	87.13	D
	2338	CG2	VAL	543	24.291	26.566	2.983	1.00	87.29	D
	2339	C	VAL	543	21.484	27.046	1.987	1.00	86.72	D
	2340	O	VAL	543	21.296	26.740	3.160	1.00	86.85	D
50	2341	N	LEU	544	20.673	26.674	1.012	1.00	86.80	D
	2342	CA	LEU	544	19.520	25.858	1.312	1.00	87.62	D
	2343	CB	LEU	544	18.229	26.624	1.018	1.00	87.72	D
55	2344	CG	LEU	544	17.996	27.129	-0.398	1.00	87.80	D
	2345	CD1	LEU	544	16.643	27.828	-0.472	1.00	86.38	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2346	CD2	LEU	544	19.120	28.074	-0.789	1.00	89.07	D
2347	C	LEU	544	19.594	24.560	0.517	1.00	88.38	D
2348	O	LEU	544	19.826	24.568	-0.700	1.00	88.44	D
2349	N	TYR	545	19.416	23.452	1.239	1.00	88.99	D
2350	CA	TYR	545	19.479	22.099	0.689	1.00	88.20	D
2351	CB	TYR	545	19.524	21.055	1.807	1.00	88.66	D
2352	CG	TYR	545	20.809	21.107	2.584	1.00	90.06	D
2353	CD1	TYR	545	20.794	21.162	3.974	1.00	90.04	D
2354	CE1	TYR	545	21.966	21.335	4.698	1.00	90.29	D
2355	CD2	TYR	545	22.040	21.210	1.927	1.00	91.31	D
2356	CE2	TYR	545	23.225	21.382	2.642	1.00	92.00	D
2357	CZ	TYR	545	23.177	21.452	4.034	1.00	91.41	D
2358	OH	TYR	545	24.319	21.694	4.770	1.00	90.69	D
2359	C	TYR	545	18.373	21.743	-0.259	1.00	87.58	D
2360	O	TYR	545	17.314	22.373	-0.286	1.00	87.17	D
2361	N	ALA	546	18.630	20.686	-1.018	1.00	87.43	D
2362	CA	ALA	546	17.706	20.212	-2.027	1.00	87.23	D
2363	CB	ALA	546	18.491	19.655	-3.188	1.00	86.89	D
2364	C	ALA	546	16.667	19.191	-1.578	1.00	87.25	D
2365	O	ALA	546	15.695	18.962	-2.292	1.00	88.37	D
2366	N	GLY	547	16.856	18.576	-0.415	1.00	86.70	D
2367	CA	GLY	547	15.893	17.580	0.027	1.00	84.97	D
2368	C	GLY	547	15.772	16.465	-1.001	1.00	84.36	D
2369	O	GLY	547	14.670	16.076	-1.389	1.00	84.24	D
2370	N	TYR	548	16.914	15.955	-1.458	1.00	83.34	D
2371	CA	TYR	548	16.942	14.882	-2.449	1.00	82.17	D
2372	CB	TYR	548	18.166	15.024	-3.364	1.00	80.47	D
2373	CG	TYR	548	18.223	14.157	-4.630	1.00	78.31	D
2374	CD1	TYR	548	17.406	14.426	-5.733	1.00	77.47	D
2375	CE1	TYR	548	17.579	13.748	-6.955	1.00	76.81	D
2376	CD2	TYR	548	19.206	13.165	-4.776	1.00	77.12	D
2377	CE2	TYR	548	19.384	12.485	-5.987	1.00	76.61	D
2378	CZ	TYR	548	18.579	12.784	-7.072	1.00	76.85	D
2379	OH	TYR	548	18.807	12.151	-8.275	1.00	76.36	D
2380	C	TYR	548	17.026	13.547	-1.740	1.00	82.76	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2381	O	TYR	548	17.520	13.440	-0.611	1.00	82.35	D
	2382	N	ASP	549	16.520	12.535	-2.419	1.00	83.15	D
10	2383	CA	ASP	549	16.562	11.184	-1.922	1.00	83.21	D
	2384	CB	ASP	549	15.230	10.485	-2.134	1.00	83.27	D
	2385	CG	ASP	549	15.216	9.110	-1.531	1.00	83.93	D
15	2386	OD1	ASP	549	16.305	8.643	-1.146	1.00	85.23	D
	2387	OD2	ASP	549	14.132	8.502	-1.443	1.00	84.20	D
	2388	C	ASP	549	17.609	10.556	-2.817	1.00	83.68	D
	2389	O	ASP	549	17.330	10.226	-3.971	1.00	83.55	D
20	2390	N	SER	550	18.821	10.430	-2.298	1.00	84.19	D
	2391	CA	SER	550	19.920	9.853	-3.054	1.00	85.11	D
	2392	CB	SER	550	21.225	10.584	-2.720	1.00	84.86	D
25	2393	OG	SER	550	21.524	10.497	-1.335	1.00	85.47	D
	2394	C	SER	550	20.028	8.384	-2.686	1.00	85.74	D
	2395	O	SER	550	21.019	7.718	-2.992	1.00	85.66	D
	2396	N	SER	551	18.982	7.897	-2.023	1.00	86.44	D
30	2397	CA	SER	551	18.902	6.515	-1.570	1.00	86.68	D
	2398	CB	SER	551	17.908	6.387	-0.431	1.00	86.76	D
	2399	OG	SER	551	16.603	6.257	-0.965	1.00	88.21	D
35	2400	C	SER	551	18.418	5.639	-2.696	1.00	86.60	D
	2401	O	SER	551	18.192	4.441	-2.527	1.00	86.16	D
	2402	N	VAL	552	18.212	6.235	-3.854	1.00	87.52	D
	2403	CA	VAL	552	17.744	5.444	-4.955	1.00	88.87	D
40	2404	CB	VAL	552	16.263	5.469	-4.935	1.00	88.89	D
	2405	CG1	VAL	552	15.800	5.509	-3.488	1.00	88.42	D
	2406	CG2	VAL	552	15.778	6.674	-5.638	1.00	88.55	D
45	2407	C	VAL	552	18.349	6.072	-6.192	1.00	89.48	D
	2408	O	VAL	552	18.434	7.303	-6.289	1.00	89.94	D
	2409	N	PRO	553	18.749	5.233	-7.166	1.00	90.53	D
	2410	CD	PRO	553	18.293	3.842	-7.338	1.00	91.20	D
50	2411	CA	PRO	553	19.382	5.726	-8.389	1.00	91.54	D
	2412	CB	PRO	553	19.267	4.570	-9.388	1.00	91.76	D
	2413	CG	PRO	553	18.260	3.673	-8.844	1.00	91.49	D
55	2414	C	PRO	553	18.968	7.021	-8.977	1.00	92.07	D
	2415	O	PRO	553	17.865	7.522	-8.784	1.00	92.26	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2416	N	ASP	554	19.915	7.570	-9.712	1.00	92.21	D
2417	CA	ASP	554	19.671	8.819	-10.342	1.00	92.25	D
2418	CB	ASP	554	20.943	9.625	-10.433	1.00	91.71	D
2419	CG	ASP	554	21.565	9.814	-9.105	1.00	91.92	D
2420	OD1	ASP	554	20.807	9.769	-8.111	1.00	92.26	D
2421	OD2	ASP	554	22.793	10.007	-9.047	1.00	91.66	D
2422	C	ASP	554	19.149	8.605	-11.701	1.00	92.49	D
2423	O	ASP	554	19.017	7.491	-12.204	1.00	93.01	D
2424	N	SER	555	18.841	9.728	-12.295	1.00	92.63	D
2425	CA	SER	555	18.365	9.750	-13.628	1.00	93.51	D
2426	CB	SER	555	17.024	9.031	-13.751	1.00	93.19	D
2427	OG	SER	555	15.938	9.844	-13.371	1.00	93.50	D
2428	C	SER	555	18.253	11.225	-13.787	1.00	94.69	D
2429	O	SER	555	17.974	11.959	-12.834	1.00	95.13	D
2430	N	THR	556	18.534	11.675	-14.992	1.00	95.90	D
2431	CA	THR	556	18.504	13.080	-15.220	1.00	96.67	D
2432	CB	THR	556	18.659	13.418	-16.575	1.00	97.22	D
2433	OG1	THR	556	19.705	12.608	-17.088	1.00	98.43	D
2434	CG2	THR	556	19.003	14.886	-16.674	1.00	97.19	D
2435	C	THR	556	17.242	13.616	-14.836	1.00	96.67	D
2436	O	THR	556	17.239	14.267	-13.831	1.00	96.78	D
2437	N	TRP	557	16.198	13.399	-15.645	1.00	97.24	D
2438	CA	TRP	557	14.885	13.878	-15.294	1.00	97.34	D
2439	CB	TRP	557	13.843	12.915	-15.846	1.00	100.14	D
2440	CG	TRP	557	13.864	13.048	-17.342	1.00	103.86	D
2441	CD2	TRP	557	13.027	12.435	-18.291	1.00	105.46	D
2442	CE2	TRP	557	13.343	12.882	-19.587	1.00	106.20	D
2443	CE3	TRP	557	11.906	11.550	-18.197	1.00	105.69	D
2444	CD1	TRP	557	14.738	13.832	-18.082	1.00	104.90	D
2445	NE1	TRP	557	14.464	13.754	-19.414	1.00	105.88	D
2446	CZ2	TRP	557	12.747	12.485	-20.763	1.00	106.15	D
2447	CZ3	TRP	557	11.277	11.129	-19.365	1.00	105.93	D
2448	CH2	TRP	557	11.674	11.619	-20.623	1.00	106.20	D
2449	C	TRP	557	15.061	13.885	-13.803	1.00	95.80	D
2450	O	TRP	557	15.879	14.624	-13.353	1.00	95.83	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2451	N	ARG	558	14.400	13.116	-12.985	1.00	93.50	D
	2452	CA	ARG	558	14.743	13.277	-11.573	1.00	91.63	D
10	2453	CB	ARG	558	15.415	12.048	-11.058	1.00	91.10	D
	2454	CG	ARG	558	15.020	11.954	-9.656	1.00	90.49	D
	2455	CD	ARG	558	14.884	10.562	-9.315	1.00	89.68	D
15	2456	NE	ARG	558	15.970	10.187	-8.440	1.00	89.44	D
	2457	CZ	ARG	558	15.933	10.373	-7.130	1.00	89.73	D
	2458	NH1	ARG	558	14.861	10.929	-6.578	1.00	88.39	D
	2459	NH2	ARG	558	16.943	9.976	-6.368	1.00	89.50	D
20	2460	C	ARG	558	15.577	14.447	-11.003	1.00	90.86	D
	2461	O	ARG	558	15.171	15.095	-10.053	1.00	90.88	D
	2462	N	ILE	559	16.756	14.695	-11.544	1.00	89.58	D
25	2463	CA	ILE	559	17.604	15.729	-10.998	1.00	88.94	D
	2464	CB	ILE	559	18.964	15.397	-11.261	1.00	88.55	D
	2465	CG2	ILE	559	19.823	16.584	-11.025	1.00	88.39	D
	2466	CG1	ILE	559	19.338	14.230	-10.403	1.00	88.44	D
30	2467	CD1	ILE	559	20.792	14.151	-10.319	1.00	88.21	D
	2468	C	ILE	559	17.438	17.109	-11.513	1.00	88.86	D
	2469	O	ILE	559	17.733	18.112	-10.853	1.00	88.86	D
35	2470	N	MET	560	17.098	17.147	-12.772	1.00	88.53	D
	2471	CA	MET	560	16.863	18.409	-13.360	1.00	88.39	D
	2472	CB	MET	560	16.426	18.226	-14.761	1.00	88.54	D
	2473	CG	MET	560	17.550	17.945	-15.603	1.00	89.76	D
40	2474	SD	MET	560	17.064	17.908	-17.282	1.00	92.87	D
	2475	CE	MET	560	18.550	18.420	-18.053	1.00	92.53	D
	2476	C	MET	560	15.653	18.747	-12.618	1.00	88.07	D
45	2477	O	MET	560	15.393	19.883	-12.229	1.00	88.78	D
	2478	N	THR	561	14.867	17.727	-12.389	1.00	86.83	D
	2479	CA	THR	561	13.682	18.152	-11.800	1.00	85.30	D
	2480	CB	THR	561	12.662	17.110	-11.851	1.00	84.89	D
50	2481	OG1	THR	561	11.788	17.422	-12.945	1.00	84.68	D
	2482	CG2	THR	561	11.909	17.094	-10.585	1.00	84.42	D
	2483	C	THR	561	13.902	18.736	-10.448	1.00	84.31	D
55	2484	O	THR	561	13.522	19.882	-10.225	1.00	84.37	D
	2485	N	THR	562	14.555	17.990	-9.569	1.00	83.16	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2486	CA	THR	562	14.833	18.504	-8.251	1.00	82.17	D
	2487	CB	THR	562	15.786	17.565	-7.420	1.00	82.07	D
10	2488	OG1	THR	562	17.047	17.455	-8.089	1.00	82.61	D
	2489	CG2	THR	562	15.185	16.154	-7.228	1.00	82.32	D
	2490	C	THR	562	15.475	19.901	-8.403	1.00	81.33	D
15	2491	O	THR	562	15.039	20.807	-7.712	1.00	82.35	D
	2492	N	LEU	563	16.442	20.097	-9.317	1.00	79.93	D
	2493	CA	LEU	563	17.134	21.413	-9.487	1.00	78.45	D
	2494	CB	LEU	563	18.268	21.323	-10.557	1.00	77.66	D
20	2495	CG	LEU	563	19.514	20.947	-9.730	1.00	78.54	D
	2496	CD1	LEU	563	18.945	20.372	-8.463	1.00	79.05	D
	2497	CD2	LEU	563	20.458	19.923	-10.336	1.00	78.61	D
25	2498	C	LEU	563	16.264	22.641	-9.693	1.00	77.89	D
	2499	O	LEU	563	16.525	23.707	-9.131	1.00	77.49	D
	2500	N	ASN	564	15.211	22.470	-10.470	1.00	77.41	D
	2501	CA	ASN	564	14.231	23.514	-10.738	1.00	76.89	D
30	2502	CB	ASN	564	13.261	23.004	-11.770	1.00	75.58	D
	2503	CG	ASN	564	13.809	23.077	-13.162	1.00	74.85	D
	2504	OD1	ASN	564	15.013	23.104	-13.393	1.00	75.81	D
35	2505	ND2	ASN	564	12.922	23.088	-14.103	1.00	75.21	D
	2506	C	ASN	564	13.465	23.900	-9.473	1.00	76.70	D
	2507	O	ASN	564	13.204	25.076	-9.222	1.00	76.62	D
	2508	N	MET	565	13.062	22.901	-8.699	1.00	77.18	D
40	2509	CA	MET	565	12.367	23.187	-7.457	1.00	77.91	D
	2510	CB	MET	565	12.112	21.901	-6.675	1.00	79.42	D
	2511	CG	MET	565	10.648	21.571	-6.452	1.00	81.29	D
45	2512	SD	MET	565	9.742	21.346	-7.996	1.00	83.79	D
	2513	CE	MET	565	8.275	22.311	-7.661	1.00	84.35	D
	2514	C	MET	565	13.367	24.047	-6.695	1.00	77.81	D
	2515	O	MET	565	13.056	25.148	-6.229	1.00	77.62	D
50	2516	N	LEU	566	14.592	23.542	-6.602	1.00	77.54	D
	2517	CA	LEU	566	15.623	24.263	-5.894	1.00	77.35	D
	2518	CB	LEU	566	16.983	23.594	-6.052	1.00	76.46	D
55	2519	CG	LEU	566	17.908	24.447	-5.190	1.00	76.14	D
	2520	CD1	LEU	566	17.281	24.541	-3.813	1.00	76.45	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2521	CD2	LEU	566	19.301	23.887	-5.113	1.00	76.14	D
	2522	C	LEU	566	15.749	25.705	-6.346	1.00	78.03	D
10	2523	O	LEU	566	15.956	26.598	-5.524	1.00	78.22	D
	2524	N	GLY	567	15.644	25.925	-7.653	1.00	78.32	D
	2525	CA	GLY	567	15.766	27.264	-8.199	1.00	78.16	D
15	2526	C	GLY	567	14.644	28.156	-7.715	1.00	78.69	D
	2527	O	GLY	567	14.853	29.334	-7.410	1.00	78.69	D
	2528	N	GLY	568	13.451	27.572	-7.658	1.00	78.97	D
	2529	CA	GLY	568	12.291	28.295	-7.192	1.00	77.68	D
20	2530	C	GLY	568	12.574	28.751	-5.785	1.00	77.16	D
	2531	O	GLY	568	12.456	29.926	-5.460	1.00	78.00	D
	2532	N	ARG	569	12.983	27.846	-4.922	1.00	75.95	D
25	2533	CA	ARG	569	13.219	28.320	-3.589	1.00	76.63	D
	2534	CB	ARG	569	13.493	27.128	-2.691	1.00	78.37	D
	2535	CG	ARG	569	12.355	26.113	-2.806	1.00	81.13	D
	2536	CD	ARG	569	12.650	24.904	-1.976	1.00	83.19	D
30	2537	NE	ARG	569	13.118	25.333	-0.668	1.00	84.03	D
	2538	CZ	ARG	569	14.210	24.856	-0.090	1.00	85.57	D
	2539	NH1	ARG	569	14.933	23.933	-0.712	1.00	85.65	D
35	2540	NH2	ARG	569	14.591	25.317	1.094	1.00	86.82	D
	2541	C	ARG	569	14.304	29.402	-3.504	1.00	76.48	D
	2542	O	ARG	569	14.198	30.301	-2.673	1.00	77.05	D
40	2543	N	GLN	570	15.307	29.353	-4.390	1.00	75.83	D
	2544	CA	GLN	570	16.409	30.332	-4.394	1.00	74.43	D
	2545	CB	GLN	570	17.633	29.763	-5.110	1.00	75.14	D
	2546	CG	GLN	570	18.513	28.845	-4.290	1.00	74.93	D
45	2547	CD	GLN	570	19.487	28.081	-5.164	1.00	74.79	D
	2548	OE1	GLN	570	20.479	27.532	-4.681	1.00	75.77	D
	2549	NE2	GLN	570	19.197	28.032	-6.463	1.00	73.98	D
50	2550	C	GLN	570	16.112	31.684	-5.026	1.00	74.13	D
	2551	O	GLN	570	16.736	32.687	-4.669	1.00	74.57	D
	2552	N	VAL	571	15.197	31.707	-5.994	1.00	72.68	D
	2553	CA	VAL	571	14.834	32.951	-6.664	1.00	71.57	D
55	2554	CB	VAL	571	14.183	32.649	-8.039	1.00	71.29	D
	2555	CG1	VAL	571	13.528	33.895	-8.630	1.00	70.57	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2556	CG2	VAL	571	15.264	32.134	-8.985	1.00	70.98	D
2557	C	VAL	571	13.911	33.739	-5.736	1.00	70.76	D
2558	O	VAL	571	13.829	34.972	-5.805	1.00	70.66	D
2559	N	ILE	572	13.244	33.004	-4.851	1.00	69.37	D
2560	CA	ILE	572	12.356	33.588	-3.860	1.00	67.55	D
2561	CB	ILE	572	11.428	32.507	-3.247	1.00	67.43	D
2562	CG2	ILE	572	11.025	32.883	-1.821	1.00	66.71	D
2563	CG1	ILE	572	10.210	32.330	-4.166	1.00	65.46	D
2564	CD1	ILE	572	9.499	31.009	-4.031	1.00	64.46	D
2565	C	ILE	572	13.246	34.234	-2.804	1.00	66.03	D
2566	O	ILE	572	12.946	35.316	-2.317	1.00	67.56	D
2567	N	ALA	573	14.355	33.588	-2.471	1.00	64.63	D
2568	CA	ALA	573	15.275	34.170	-1.501	1.00	64.65	D
2569	CB	ALA	573	16.281	33.116	-1.028	1.00	64.20	D
2570	C	ALA	573	16.009	35.348	-2.159	1.00	65.16	D
2571	O	ALA	573	16.571	36.213	-1.466	1.00	63.91	D
2572	N	ALA	574	15.980	35.367	-3.499	1.00	65.57	D
2573	CA	ALA	574	16.626	36.403	-4.334	1.00	65.65	D
2574	CB	ALA	574	16.706	35.916	-5.791	1.00	64.41	D
2575	C	ALA	574	15.873	37.732	-4.267	1.00	65.77	D
2576	O	ALA	574	16.442	38.816	-4.435	1.00	64.59	D
2577	N	VAL	575	14.572	37.624	-4.037	1.00	66.30	D
2578	CA	VAL	575	13.717	38.774	-3.916	1.00	67.41	D
2579	CB	VAL	575	12.261	38.365	-4.194	1.00	67.80	D
2580	CG1	VAL	575	11.342	39.580	-4.126	1.00	66.72	D
2581	CG2	VAL	575	12.183	37.695	-5.572	1.00	68.22	D
2582	C	VAL	575	13.903	39.353	-2.500	1.00	68.51	D
2583	O	VAL	575	14.030	40.573	-2.363	1.00	68.32	D
2584	N	LYS	576	13.937	38.516	-1.448	1.00	68.40	D
2585	CA	LYS	576	14.159	39.085	-0.103	1.00	69.53	D
2586	CB	LYS	576	14.044	38.055	1.073	1.00	72.11	D
2587	CG	LYS	576	12.641	37.402	1.379	1.00	77.34	D
2588	CD	LYS	576	12.456	36.763	2.842	1.00	80.60	D
2589	CE	LYS	576	13.443	35.602	3.211	1.00	83.74	D
2590	NZ	LYS	576	13.115	34.750	4.436	1.00	83.62	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2591	C	LYS	576	15.593	39.643	-0.132	1.00	68.77	D
	2592	O	LYS	576	15.895	40.648	0.514	1.00	70.13	D
10	2593	N	TRP	577	16.489	39.007	-0.878	1.00	66.43	D
	2594	CA	TRP	577	17.842	39.536	-0.913	1.00	63.78	D
	2595	CB	TRP	577	18.790	38.561	-1.620	1.00	61.85	D
15	2596	CG	TRP	577	20.107	39.167	-1.989	1.00	58.40	D
	2597	CD2	TRP	577	20.517	39.533	-3.302	1.00	57.61	D
	2598	CE2	TRP	577	21.836	40.028	-3.210	1.00	57.50	D
	2599	CE3	TRP	577	19.920	39.441	-4.565	1.00	56.82	D
20	2600	CD1	TRP	577	21.136	39.486	-1.158	1.00	57.68	D
	2601	NE1	TRP	577	22.182	40.009	-1.884	1.00	58.31	D
	2602	CZ2	TRP	577	22.542	40.486	-4.322	1.00	57.43	D
25	2603	CZ3	TRP	577	20.617	39.894	-5.668	1.00	56.94	D
	2604	CH2	TRP	577	21.928	40.389	-5.545	1.00	57.05	D
	2605	C	TRP	577	17.856	40.901	-1.609	1.00	62.95	D
	2606	O	TRP	577	18.328	41.881	-1.035	1.00	61.99	D
30	2607	N	ALA	578	17.324	40.959	-2.826	1.00	62.89	D
	2608	CA	ALA	578	17.288	42.201	-3.610	1.00	63.57	D
	2609	CB	ALA	578	16.480	41.988	-4.895	1.00	62.98	D
35	2610	C	ALA	578	16.724	43.380	-2.821	1.00	64.15	D
	2611	O	ALA	578	17.341	44.446	-2.769	1.00	63.71	D
	2612	N	LYS	579	15.557	43.178	-2.213	1.00	64.96	D
	2613	CA	LYS	579	14.901	44.196	-1.406	1.00	65.52	D
40	2614	CB	LYS	579	13.617	43.610	-0.812	1.00	67.19	D
	2615	CG	LYS	579	12.524	43.330	-1.856	1.00	68.64	D
	2616	CD	LYS	579	11.399	42.409	-1.353	1.00	69.03	D
45	2617	CE	LYS	579	11.014	42.666	0.106	1.00	69.80	D
	2618	NZ	LYS	579	9.561	42.402	0.366	1.00	70.70	D
	2619	C	LYS	579	15.809	44.754	-0.293	1.00	65.43	D
	2620	O	LYS	579	15.728	45.933	0.044	1.00	65.59	D
50	2621	N	ALA	580	16.687	43.930	0.264	1.00	64.59	D
	2622	CA	ALA	580	17.577	44.407	1.325	1.00	64.93	D
	2623	CB	ALA	580	18.038	43.234	2.192	1.00	65.44	D
55	2624	C	ALA	580	18.793	45.178	0.817	1.00	64.74	D
	2625	O	ALA	580	19.532	45.780	1.604	1.00	64.88	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2626	N	ILE	581	19.013	45.157	-0.492	1.00	64.45	D
	2627	CA	ILE	581	20.152	45.867	-1.048	1.00	64.93	D
10	2628	CB	ILE	581	20.382	45.492	-2.515	1.00	63.01	D
	2629	CG2	ILE	581	21.375	46.449	-3.160	1.00	62.56	D
	2630	CG1	ILE	581	20.908	44.068	-2.592	1.00	60.84	D
	2631	CD1	ILE	581	20.782	43.502	-3.944	1.00	59.17	D
15	2632	C	ILE	581	19.916	47.364	-0.949	1.00	66.48	D
	2633	O	ILE	581	18.937	47.900	-1.473	1.00	67.02	D
	2634	N	PRO	582	20.806	48.055	-0.238	1.00	67.71	D
20	2635	CD	PRO	582	21.885	47.468	0.572	1.00	68.94	D
	2636	CA	PRO	582	20.747	49.499	-0.039	1.00	69.60	D
	2637	CB	PRO	582	22.138	49.810	0.481	1.00	69.24	D
	2638	CG	PRO	582	22.394	48.676	1.353	1.00	69.39	D
25	2639	C	PRO	582	20.452	50.200	-1.349	1.00	70.14	D
	2640	O	PRO	582	21.234	50.111	-2.296	1.00	70.73	D
	2641	N	GLY	583	19.318	50.885	-1.408	1.00	70.94	D
30	2642	CA	GLY	583	18.947	51.599	-2.611	1.00	72.37	D
	2643	C	GLY	583	18.149	50.832	-3.652	1.00	74.21	D
	2644	O	GLY	583	17.795	51.397	-4.676	1.00	74.83	D
	2645	N	PHE	584	17.844	49.555	-3.422	1.00	74.85	D
35	2646	CA	PHE	584	17.092	48.813	-4.429	1.00	74.38	D
	2647	CB	PHE	584	17.361	47.309	-4.321	1.00	70.65	D
	2648	CG	PHE	584	16.647	46.498	-5.369	1.00	67.79	D
40	2649	CD1	PHE	584	17.111	46.468	-6.684	1.00	65.83	D
	2650	CD2	PHE	584	15.470	45.821	-5.056	1.00	66.67	D
	2651	CE1	PHE	584	16.404	45.783	-7.677	1.00	63.42	D
45	2652	CE2	PHE	584	14.756	45.138	-6.039	1.00	65.18	D
	2653	CZ	PHE	584	15.225	45.120	-7.353	1.00	64.10	D
	2654	C	PHE	584	15.587	49.053	-4.351	1.00	76.56	D
	2655	O	PHE	584	14.924	49.153	-5.385	1.00	76.30	D
50	2656	N	ARG	585	15.058	49.140	-3.131	1.00	79.68	D
	2657	CA	ARG	585	13.620	49.343	-2.898	1.00	81.83	D
	2658	CB	ARG	585	13.277	49.230	-1.404	1.00	82.57	D
55	2659	CG	ARG	585	13.320	47.822	-0.844	1.00	85.17	D
	2660	CD	ARG	585	12.282	47.604	0.253	1.00	87.14	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2661	NE	ARG	585	10.921	47.879	-0.208	1.00	89.83	D
	2662	CZ	ARG	585	10.378	47.395	-1.327	1.00	90.53	D
10	2663	NH1	ARG	585	11.073	46.596	-2.130	1.00	89.47	D
	2664	NH2	ARG	585	9.130	47.717	-1.650	1.00	90.67	D
	2665	C	ARG	585	13.105	50.680	-3.394	1.00	82.68	D
15	2666	O	ARG	585	11.961	50.800	-3.841	1.00	82.83	D
	2667	N	ASN	586	13.957	51.689	-3.302	1.00	83.37	D
	2668	CA	ASN	586	13.582	53.021	-3.717	1.00	84.07	D
	2669	CB	ASN	586	14.559	54.021	-3.111	1.00	85.16	D
20	2670	CG	ASN	586	14.559	53.959	-1.593	1.00	86.57	D
	2671	OD1	ASN	586	15.605	53.793	-0.958	1.00	86.08	D
	2672	ND2	ASN	586	13.368	54.076	-1.004	1.00	87.02	D
25	2673	C	ASN	586	13.482	53.180	-5.218	1.00	83.72	D
	2674	O	ASN	586	13.251	54.274	-5.715	1.00	84.47	D
	2675	N	LEU	587	13.668	52.105	-5.963	1.00	83.66	D
	2676	CA	LEU	587	13.506	52.244	-7.394	1.00	83.96	D
30	2677	CB	LEU	587	14.377	51.266	-8.177	1.00	82.49	D
	2678	CG	LEU	587	15.893	51.449	-8.222	1.00	80.62	D
	2679	CD1	LEU	587	16.502	50.072	-8.268	1.00	80.84	D
35	2680	CD2	LEU	587	16.339	52.269	-9.424	1.00	78.79	D
	2681	C	LEU	587	12.049	51.908	-7.606	1.00	85.36	D
	2682	O	LEU	587	11.378	51.373	-6.721	1.00	85.16	D
	2683	N	HIS	588	11.561	52.223	-8.792	1.00	86.53	D
40	2684	CA	HIS	588	10.186	51.949	-9.110	1.00	87.58	D
	2685	CB	HIS	588	9.908	52.395	-10.533	1.00	88.54	D
	2686	CG	HIS	588	8.461	52.636	-10.806	1.00	90.27	D
45	2687	CD2	HIS	588	7.739	53.783	-10.820	1.00	90.56	D
	2688	ND1	HIS	588	7.567	51.616	-11.046	1.00	90.27	D
	2689	CE1	HIS	588	6.358	52.122	-11.200	1.00	90.42	D
	2690	NE2	HIS	588	6.437	53.436	-11.068	1.00	90.75	D
50	2691	C	HIS	588	9.900	50.461	-8.957	1.00	87.99	D
	2692	O	HIS	588	10.651	49.636	-9.464	1.00	88.40	D
	2693	N	LEU	589	8.821	50.129	-8.260	1.00	88.47	D
55	2694	CA	LEU	589	8.421	48.740	-8.052	1.00	88.53	D
	2695	CB	LEU	589	7.093	48.679	-7.306	1.00	88.25	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2696	CG	LEU	589	6.842	47.395	-6.527	1.00	89.05	D
2697	CD1	LEU	589	6.931	47.743	-5.056	1.00	89.76	D
2698	CD2	LEU	589	5.482	46.787	-6.860	1.00	88.71	D
2699	C	LEU	589	8.256	48.003	-9.382	1.00	88.65	D
2700	O	LEU	589	7.991	46.803	-9.407	1.00	88.78	D
2701	N	ASP	590	8.396	48.735	-10.483	1.00	88.97	D
2702	CA	ASP	590	8.269	48.163	-11.819	1.00	89.67	D
2703	CB	ASP	590	7.587	49.166	-12.758	1.00	91.42	D
2704	CG	ASP	590	6.149	48.786	-13.080	1.00	92.34	D
2705	OD1	ASP	590	5.466	48.223	-12.196	1.00	93.01	D
2706	OD2	ASP	590	5.702	49.064	-14.217	1.00	93.07	D
2707	C	ASP	590	9.641	47.794	-12.365	1.00	89.21	D
2708	O	ASP	590	9.766	46.872	-13.174	1.00	89.72	D
2709	N	ASP	591	10.663	48.528	-11.941	1.00	88.41	D
2710	CA	ASP	591	12.033	48.252	-12.365	1.00	87.48	D
2711	CB	ASP	591	12.925	49.470	-12.157	1.00	89.21	D
2712	CG	ASP	591	12.417	50.683	-12.885	1.00	90.55	D
2713	OD1	ASP	591	11.775	50.505	-13.943	1.00	91.32	D
2714	OD2	ASP	591	12.670	51.811	-12.407	1.00	90.79	D
2715	C	ASP	591	12.514	47.125	-11.480	1.00	85.89	D
2716	O	ASP	591	13.210	46.213	-11.928	1.00	85.48	D
2717	N	GLN	592	12.132	47.227	-10.208	1.00	84.16	D
2718	CA	GLN	592	12.450	46.231	-9.204	1.00	82.32	D
2719	CB	GLN	592	11.654	46.496	-7.914	1.00	81.57	D
2720	CG	GLN	592	12.383	47.381	-6.904	1.00	82.24	D
2721	CD	GLN	592	11.593	47.633	-5.622	1.00	82.59	D
2722	OE1	GLN	592	11.225	46.704	-4.896	1.00	82.42	D
2723	NE2	GLN	592	11.340	48.905	-5.332	1.00	83.09	D
2724	C	GLN	592	12.046	44.891	-9.790	1.00	81.43	D
2725	O	GLN	592	12.658	43.863	-9.513	1.00	81.40	D
2726	N	MET	593	11.014	44.913	-10.625	1.00	80.58	D
2727	CA	MET	593	10.529	43.694	-11.249	1.00	79.77	D
2728	CB	MET	593	9.027	43.756	-11.480	1.00	81.53	D
2729	CG	MET	593	8.224	43.102	-10.394	1.00	83.90	D
2730	SD	MET	593	6.539	42.873	-10.938	1.00	86.70	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2731	CE	MET	593	5.819	44.357	-10.312	1.00	86.41	D
	2732	C	MET	593	11.189	43.379	-12.563	1.00	78.53	D
10	2733	O	MET	593	11.140	42.234	-13.012	1.00	78.60	D
	2734	N	THR	594	11.784	44.377	-13.208	1.00	76.34	D
	2735	CA	THR	594	12.429	44.086	-14.476	1.00	74.92	D
15	2736	CB	THR	594	12.608	45.340	-15.353	1.00	75.23	D
	2737	OG1	THR	594	11.648	46.336	-14.979	1.00	75.76	D
	2738	CG2	THR	594	12.388	44.976	-16.822	1.00	74.71	D
	2739	C	THR	594	13.798	43.504	-14.174	1.00	73.12	D
20	2740	O	THR	594	14.198	42.481	-14.741	1.00	72.69	D
	2741	N	LEU	595	14.498	44.156	-13.255	1.00	70.86	D
	2742	CA	LEU	595	15.822	43.721	-12.869	1.00	68.87	D
25	2743	CB	LEU	595	16.363	44.672	-11.783	1.00	67.46	D
	2744	CG	LEU	595	16.546	46.137	-12.248	1.00	65.81	D
	2745	CD1	LEU	595	17.104	46.982	-11.111	1.00	65.46	D
	2746	CD2	LEU	595	17.484	46.212	-13.454	1.00	64.25	D
30	2747	C	LEU	595	15.837	42.233	-12.444	1.00	68.29	D
	2748	O	LEU	595	16.655	41.460	-12.945	1.00	67.78	D
	2749	N	LEU	596	14.919	41.815	-11.571	1.00	67.24	D
35	2750	CA	LEU	596	14.867	40.417	-11.145	1.00	66.35	D
	2751	CB	LEU	596	13.898	40.242	-10.015	1.00	64.75	D
	2752	CG	LEU	596	14.549	40.758	-8.763	1.00	65.03	D
	2753	CD1	LEU	596	13.510	40.709	-7.689	1.00	65.87	D
40	2754	CD2	LEU	596	15.772	39.920	-8.402	1.00	63.70	D
	2755	C	LEU	596	14.450	39.468	-12.223	1.00	67.95	D
	2756	O	LEU	596	14.648	38.260	-12.121	1.00	68.48	D
45	2757	N	GLN	597	13.834	40.003	-13.256	1.00	70.46	D
	2758	CA	GLN	597	13.385	39.144	-14.322	1.00	71.83	D
	2759	CB	GLN	597	12.092	39.680	-14.893	1.00	74.64	D
	2760	CG	GLN	597	10.889	39.131	-14.174	1.00	77.64	D
50	2761	CD	GLN	597	9.690	40.015	-14.335	1.00	80.72	D
	2762	OE1	GLN	597	9.518	40.672	-15.371	1.00	81.13	D
	2763	NE2	GLN	597	8.839	40.040	-13.312	1.00	82.34	D
55	2764	C	GLN	597	14.433	39.010	-15.389	1.00	71.17	D
	2765	O	GLN	597	14.538	37.981	-16.054	1.00	70.16	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2766	N	TYR	598	15.222	40.060	-15.547	1.00	71.62	D
	2767	CA	TYR	598	16.282	40.034	-16.530	1.00	73.19	D
10	2768	CB	TYR	598	16.699	41.442	-16.884	1.00	75.94	D
	2769	CG	TYR	598	15.858	42.139	-17.912	1.00	78.54	D
	2770	CD1	TYR	598	14.469	42.030	-17.920	1.00	79.49	D
15	2771	CE1	TYR	598	13.705	42.761	-18.828	1.00	80.77	D
	2772	CD2	TYR	598	16.459	42.988	-18.832	1.00	79.85	D
	2773	CE2	TYR	598	15.718	43.719	-19.729	1.00	80.37	D
	2774	CZ	TYR	598	14.350	43.607	-19.726	1.00	80.56	D
20	2775	OH	TYR	598	13.651	44.360	-20.628	1.00	81.35	D
	2776	C	TYR	598	17.509	39.318	-15.991	1.00	72.98	D
	2777	O	TYR	598	18.318	38.818	-16.761	1.00	73.46	D
25	2778	N	SER	599	17.653	39.246	-14.671	1.00	71.89	D
	2779	CA	SER	599	18.855	38.629	-14.141	1.00	70.45	D
	2780	CB	SER	599	19.754	39.726	-13.554	1.00	70.74	D
	2781	OG	SER	599	19.116	40.418	-12.498	1.00	71.65	D
30	2782	C	SER	599	18.773	37.475	-13.152	1.00	69.27	D
	2783	O	SER	599	19.778	37.130	-12.543	1.00	69.11	D
	2784	N	TRP	600	17.620	36.846	-12.991	1.00	68.14	D
35	2785	CA	TRP	600	17.553	35.758	-12.021	1.00	66.50	D
	2786	CB	TRP	600	16.104	35.228	-11.880	1.00	64.24	D
	2787	CG	TRP	600	15.610	34.419	-13.029	1.00	62.65	D
	2788	CD2	TRP	600	15.688	32.996	-13.158	1.00	62.35	D
40	2789	CE2	TRP	600	15.247	32.668	-14.461	1.00	62.55	D
	2790	CE3	TRP	600	16.088	31.963	-12.298	1.00	61.35	D
	2791	CD1	TRP	600	15.129	34.887	-14.220	1.00	62.62	D
45	2792	NE1	TRP	600	14.913	33.842	-15.086	1.00	62.81	D
	2793	CZ2	TRP	600	15.205	31.350	-14.928	1.00	62.62	D
	2794	CZ3	TRP	600	16.046	30.648	-12.763	1.00	61.50	D
	2795	CH2	TRP	600	15.607	30.356	-14.070	1.00	62.18	D
50	2796	C	TRP	600	18.545	34.604	-12.305	1.00	66.75	D
	2797	O	TRP	600	19.058	33.988	-11.365	1.00	66.87	D
	2798	N	MET	601	18.847	34.327	-13.576	1.00	65.69	D
55	2799	CA	MET	601	19.759	33.225	-13.902	1.00	64.40	D
	2800	CB	MET	601	19.572	32.783	-15.357	1.00	65.00	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2801	CG	MET	601	20.405	31.563	-15.746	1.00	64.60	D
	2802	SD	MET	601	19.781	30.024	-15.098	1.00	63.03	D
10	2803	CE	MET	601	18.606	29.722	-16.311	1.00	63.59	D
	2804	C	MET	601	21.216	33.612	-13.676	1.00	63.06	D
	2805	O	MET	601	22.030	32.811	-13.209	1.00	61.71	D
15	2806	N	SER	602	21.531	34.849	-14.033	1.00	62.11	D
	2807	CA	SER	602	22.858	35.392	-13.847	1.00	60.77	D
	2808	CB	SER	602	22.879	36.826	-14.363	1.00	61.16	D
	2809	OG	SER	602	24.160	37.417	-14.248	1.00	65.49	D
20	2810	C	SER	602	23.113	35.321	-12.340	1.00	59.92	D
	2811 1	O	SER	602	24.177	34.898	-11.900	1.00	58.97	D
	2812	N	LEU	603	22.111	35.709	-11.548	1.00	59.96	D
25	2813	CA	LEU	603	22.215	35.657	-10.088	1.00	60.03	D
	2814	CB	LEU	603	20.967	36.270	-9.451	1.00	59.15	D
	2815	CG	LEU	603	20.845	37.787	-9.443	1.00	58.29	D
	2816	CD1	LEU	603	19.555	38.185	-8.783	1.00	59.06	D
30	2817	CD2	LEU	603	22.015	38.374	-8.704	1.00	59.29	D
	2818	C	LEU	603	22.367	34.218	-9.556	1.00	60.99	D
	2819	O	LEU	603	23.199	33.949	-8.671	1.00	59.56	D
35	2820	N	MET	604	21.544	33.317	-10.092	1.00	61.05	D
	2821	CA	MET	604	21.535	31.914	-9.701	1.00	61.42	D
	2822	CB	MET	604	20.301	31.212	-10.291	1.00	62.57	D
	2823	CG	MET	604	18.977	31.722	-9.720	1.00	63.60	D
40	2824	SD	MET	604	18.923	31.632	-7.902	1.00	66.37	D
	2825	CE	MET	604	19.713	33.227	-7.348	1.00	61.36	D
	2826	C	MET	604	22.818	31.186	-10.104	1.00	61.75	D
45	2827	O	MET	604	23.401	30.451	-9.303	1.00	63.54	D
	2828	N	ALA	605	23.259	31.396	-11.343	1.00	61.11	D
	2829	CA	ALA	605	24.484	30.759	-11.826	1.00	58.27	D
	2830	CB	ALA	605	24.652	30.980	-13.328	1.00	56.44	D
50	2831	C	ALA	605	25.693	31.308	-11.081	1.00	57.37	D
	2832	O	ALA	605	26.508	30.533	-10.584	1.00	58.59	D
	2833	N	PHE	606	25.816	32.632	-10.982	1.00	55.71	D
55	2834	CA	PHE	606	26.969	33.185	-10.289	1.00	54.38	D
	2835	CB	PHE	606	26.883	34.693	-10.154	1.00	53.77	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2836	CG	PHE	606	28.211	35.350	-9.951	1.00	52.02	D
2837	CD1	PHE	606	29.221	35.169	-10.889	1.00	50.21	D
2838	CD2	PHE	606	28.464	36.127	-8.818	1.00	51.90	D
2839	CE1	PHE	606	30.454	35.765	-10.725	1.00	50.29	D
2840	CE2	PHE	606	29.697	36.732	-8.636	1.00	50.51	D
2841	CZ	PHE	606	30.699	36.545	-9.591	1.00	51.66	D
2842	C	PHE	606	27.121	32.578	-8.907	1.00	55.10	D
2843	O	PHE	606	28.213	32.161	-8.539	1.00	55.15	D
2844	N	ALA	607	26.039	32.527	-8.134	1.00	55.44	D
2845	CA	ALA	607	26.102	31.931	-6.805	1.00	54.39	D
2846	CB	ALA	607	24.742	31.971	-6.134	1.00	54.87	D
2847	C	ALA	607	26.618	30.484	-6.876	1.00	54.05	D
2848	O	ALA	607	27.568	30.149	-6.172	1.00	53.71	D
2849	N	LEU	608	26.015	29.628	-7.702	1.00	52.77	D
2850	CA	LEU	608	26.504	28.249	-7.822	1.00	54.52	D
2851	CB	LEU	608	25.737	27.488	-8.918	1.00	53.99	D
2852	CG	LEU	608	26.095	26.110	-9.530	1.00	53.37	D
2853	CD1	LEU	608	25.505	24.894	-8.789	1.00	52.75	D
2854	CD2	LEU	608	25.500	26.137	-10.928	1.00	51.27	D
2855	C	LEU	608	27.997	28.321	-8.167	1.00	55.73	D
2856	O	LEU	608	28.820	27.621	-7.574	1.00	55.83	D
2857	N	GLY	609	28.352	29.177	-9.119	1.00	56.30	D
2858	CA	GLY	609	29.750	29.289	-9.466	1.00	55.84	D
2859	C	GLY	609	30.519	29.339	-8.169	1.00	56.33	D
2860	O	GLY	609	31.360	28.493	-7.891	1.00	58.34	D
2861	N	TRP	610	30.194	30.320	-7.348	1.00	56.64	D
2862	CA	TRP	610	30.837	30.510	-6.063	1.00	56.47	D
2863	CB	TRP	610	30.164	31.686	-5.382	1.00	54.87	D
2864	CG	TRP	610	30.715	31.983	-4.082	1.00	54.25	D
2865	CD2	TRP	610	31.922	32.688	-3.819	1.00	54.11	D
2866	CE2	TRP	610	32.062	32.760	-2.413	1.00	53.58	D
2867	CE3	TRP	610	32.924	33.244	-4.630	1.00	54.73	D
2868	CD1	TRP	610	30.168	31.670	-2.872	1.00	53.99	D
2869	NE1	TRP	610	30.971	32.139	-1.861	1.00	52.96	D
2870	CZ2	TRP	610	33.145	33.398	-1.798	1.00	53.93	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2871	CZ3	TRP	610	34.006	33.879	-4.020	1.00	55.04	D
	2872	CH2	TRP	610	34.109	33.941	-2.614	1.00	54.37	D
10	2873	C	TRP	610	30.861	29.278	-5.126	1.00	56.15	D
	2874	O	TRP	610	31.909	28.875	-4.650	1.00	55.81	D
	2875	N	ARG	611	29.709	28.696	-4.850	1.00	57.57	D
15	2876	CA	ARG	611	29.642	27.532	-3.979	1.00	60.30	D
	2877	CB	ARG	611	28.205	27.011	-3.916	1.00	60.79	D
	2878	CG	ARG	611	27.260	27.895	-3.152	1.00	61.01	D
	2879	CD	ARG	611	26.050	27.105	-2.743	1.00	62.23	D
20	2880	NE	ARG	611	25.221	26.733	-3.885	1.00	65.70	D
	2881	CZ	ARG	611	24.575	27.609	-4.658	1.00	67.49	D
	2882	NH1	ARG	611	24.672	28.915	-4.411	1.00	67.58	D
25	2883	NH2	ARG	611	23.815	27.175	-5.662	1.00	67.11	D
	2884	C	ARG	611	30.557	26.396	-4.437	1.00	62.21	D
	2885	O	ARG	611	31.111	25.658	-3.619	1.00	62.76	D
	2886	N	SER	612	30.700	26.267	-5.752	1.00	63.60	D
30	2887	CA	SER	612	31.515	25.235	-6.376	1.00	64.24	D
	2888	CB	SER	612	31.249	25.222	-7.871	1.00	63.20	D
	2889	OG	SER	612	29.893	24.903	-8.109	1.00	64.79	D
35	2890	C	SER	612	32.992	25.440	-6.165	1.00	65.94	D
	2891	O	SER	612	33.743	24.518	-5.849	1.00	66.25	D
	2892	N	TYR	613	33.395	26.674	-6.379	1.00	67.61	D
40	2893	CA	TYR	613	34.766	27.065	-6.253	1.00	70.25	D
	2894	CB	TYR	613	34.877	28.493	-6.765	1.00	68.40	D
	2895	CG	TYR	613	35.904	29.345	-6.083	1.00	66.72	D
	2896	CD1	TYR	613	37.257	29.017	-6.129	1.00	66.00	D
45	2897	CE1	TYR	613	38.216	29.854	-5.587	1.00	65.63	D
	2898	CD2	TYR	613	35.529	30.534	-5.465	1.00	65.87	D
	2899	CE2	TYR	613	36.478	31.385	-4.920	1.00	66.64	D
50	2900	CZ	TYR	613	37.824	31.042	-4.986	1.00	66.27	D
	2901	OH	TYR	613	38.779	31.900	-4.487	1.00	66.46	D
	2902	C	TYR	613	35.274	26.960	-4.833	1.00	73.21	D
	2903	O	TYR	613	36.445	26.684	-4.603	1.00	74.48	D
55	2904	N	ARG	614	34.403	27.146	-3.862	1.00	76.37	D
	2905	CA	ARG	614	34.881	27.117	-2.496	1.00	80.08	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2906	CB	ARG	614	34.064	28.077	-1.675	1.00	81.71	D
	2907	CG	ARG	614	34.106	29.440	-2.230	1.00	84.04	D
10	2908	CD	ARG	614	34.100	30.368	-1.095	1.00	85.85	D
	2909	NE	ARG	614	35.334	31.126	-1.078	1.00	88.32	D
	2910	CZ	ARG	614	35.980	31.443	0.033	1.00	90.04	D
	2911	NH1	ARG	614	35.501	31.042	1.207	1.00	90.01	D
15	2912	NH2	ARG	614	37.086	32.173	-0.031	1.00	90.37	D
	2913	C	ARG	614	34.884	25.786	-1.798	1.00	82.06	D
	2914	O	ARG	614	35.673	25.558	-0.881	1.00	81.66	D
20	2915	N	GLN	615	33.996	24.919	-2.257	1.00	84.29	D
	2916	CA	GLN	615	33.783	23.607	-1.683	1.00	86.72	D
	2917	CB	GLN	615	32.291	23.295	-1.776	1.00	87.00	D
25	2918	CG	GLN	615	31.757	22.321	-0.758	1.00	87.90	D
	2919	CD	GLN	615	30.383	21.805	-1.139	1.00	88.85	D
	2920	OE1	GLN	615	29.469	22.583	-1.439	1.00	89.58	D
	2921	NE2	GLN	615	30.230	20.486	-1.129	1.00	88.70	D
	2922	C	GLN	615	34.570	22.480	-2.330	1.00	88.12	D
30	2923	O	GLN	615	34.636	21.376	-1.793	1.00	88.63	D
	2924	N	SER	616	35.154	22.743	-3.493	1.00	89.98	D
	2925	CA	SER	616	35.897	21.714	-4.201	1.00	92.24	D
35	2926	CB	SER	616	34.935	20.628	-4.707	1.00	91.52	D
	2927	OG	SER	616	33.666	21.166	-5.037	1.00	90.46	D
	2928	C	SER	616	36.699	22.297	-5.351	1.00	94.27	D
40	2929	O	SER	616	36.747	21.737	-6.454	1.00	94.33	D
	2930	N	SER	617	37.288	23.457	-5.076	1.00	96.24	D
	2931	CA	SER	617	38.160	24.176	-5.995	1.00	98.57	D
45	2932	CB	SER	617	39.554	23.553	-5.872	1.00	99.03	D
	2933	OG	SER	617	39.571	22.606	-4.807	1.00	99.55	D
	2934	C	SER	617	37.755	24.286	-7.482	1.00	99.70	D
	2935	O	SER	617	38.627	24.410	-8.349	1.00	100.43	D
	2936	N	ALA	618	36.451	24.269	-7.761	1.00	99.99	D
50	2937	CA	ALA	618	35.910	24.355	-9.129	1.00	100.55	D
	2938	CB	ALA	618	36.607	25.472	-9.927	1.00	100.28	D
	2939	C	ALA	618	36.023	23.019	-9.877	1.00	101.11	D
55	2940	O	ALA	618	36.252	22.988	-11.095	1.00	102.13	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	2941	N	ASN	619	35.846	21.925	-9.140	1.00	100.05	D
	2942	CA	ASN	619	35.920	20.572	-9.686	1.00	98.66	D
10	2943	CB	ASN	619	36.717	19.698	-8.729	1.00	98.89	D
	2944	CG	ASN	619	38.173	20.061	-8.710	1.00	99.76	D
	2945	OD1	ASN	619	38.989	19.409	-9.362	1.00	100.38	D
15	2946	ND2	ASN	619	38.513	21.118	-7.984	1.00	100.19	D
	2947	C	ASN	619	34.537	19.956	-9.898	1.00	97.79	D
	2948	O	ASN	619	34.263	19.341	-10.933	1.00	97.87	D
	2949	N	LEU	620	33.689	20.138	-8.889	1.00	95.84	D
20	2950	CA	LEU	620	32.311	19.639	-8.847	1.00	93.00	D
	2951	CB	LEU	620	32.115	18.877	-7.520	1.00	92.86	D
	2952	CG	LEU	620	32.410	17.366	-7.399	1.00	93.21	D
25	2953	CD1	LEU	620	33.616	16.984	-8.224	1.00	93.46	D
	2954	CD2	LEU	620	32.620	16.984	-5.936	1.00	93.04	D
	2955	C	LEU	620	31.305	20.815	-8.945	1.00	90.83	D
	2956	O	LEU	620	31.656	21.951	-8.634	1.00	90.07	D
30	2957	N	LEU	621	30.080	20.559	-9.417	1.00	88.70	D
	2958	CA	LEU	621	29.042	21.602	-9.478	1.00	86.58	D
	2959	CB	LEU	621	28.116	21.448	-10.702	1.00	85.41	D
35	2960	CG	LEU	621	28.548	22.141	-12.005	1.00	84.56	D
	2961	CD1	LEU	621	27.426	22.091	-13.034	1.00	83.62	D
	2962	CD2	LEU	621	28.920	23.591	-11.705	1.00	83.64	D
	2963	C	LEU	621	28.257	21.351	-8.201	1.00	85.65	D
40	2964	O	LEU	621	27.712	20.267	-8.015	1.00	84.66	D
	2965	N	CYS	622	28.195	22.352	-7.329	1.00	84.99	D
	2966	CA	CYS	622	27.547	22.173	-6.033	1.00	84.82	D
45	2967	CB	CYS	622	28.555	22.513	-4.943	1.00	84.44	D
	2968	SG	CYS	622	30.165	21.733	-5.213	1.00	84.00	D
	2969	C	CYS	622	26.256	22.923	-5.775	1.00	85.04	D
	2970	O	CYS	622	26.237	23.915	-5.046	1.00	85.22	D
50	2971	N	PHE	623	25.166	22.418	-6.321	1.00	85.24	D
	2972	CA	PHE	623	23.879	23.058	-6.161	1.00	85.95	D
	2973	CB	PHE	623	22.842	22.244	-6.917	1.00	84.99	D
55	2974	CG	PHE	623	23.133	22.232	-8.381	1.00	84.67	D
	2975	CD1	PHE	623	24.170	21.456	-8.896	1.00	84.97	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2976	CD2	PHE	623	22.378	22.995	-9.256	1.00	84.22	D
2977	CE1	PHE	623	24.531	21.545	-10.242	1.00	84.00	D
2978	CE2	PHE	623	22.733	23.093	-10.600	1.00	83.93	D
2979	CZ	PHE	623	23.779	22.324	-11.103	1.00	84.03	D
2980	C	PHE	623	23.451	23.362	-4.722	1.00	87.69	D
2981	O	PHE	623	23.098	24.506	-4.424	1.00	87.48	D
2982	N	ALA	624	23.492	22.364	-3.844	1.00	89.72	D
2983	CA	ALA	624	23.135	22.522	-2.422	1.00	91.56	D
2984	CB	ALA	624	21.650	22.219	-2.214	1.00	91.67	D
2985	C	ALA	624	23.989	21.484	-1.693	1.00	92.97	D
2986	O	ALA	624	23.729	20.308	-1.854	1.00	93.10	D
2987	N	PRO	625	25.007	21.894	-0.893	1.00	94.78	D
2988	CD	PRO	625	25.468	23.245	-0.512	1.00	95.11	D
2989	CA	PRO	625	25.824	20.873	-0.211	1.00	95.23	D
2990	CB	PRO	625	26.256	21.600	1.061	1.00	95.14	D
2991	CG	PRO	625	26.614	22.958	0.500	1.00	94.67	D
2992	C	PRO	625	25.285	19.441	0.026	1.00	94.97	D
2993	O	PRO	625	26.069	18.542	0.330	1.00	95.36	D
2994	N	ASP	626	23.970	19.242	-0.116	1.00	94.20	D
2995	CA	ASP	626	23.327	17.927	-0.008	1.00	93.55	D
2996	CB	ASP	626	21.992	18.026	0.797	1.00	95.17	D
2997	CG	ASP	626	20.697	17.895	-0.073	1.00	96.51	D
2998	OD1	ASP	626	20.722	18.077	-1.311	1.00	96.93	D
2999	OD2	ASP	626	19.616	17.628	0.506	1.00	97.12	D
3000	C	ASP	626	23.083	17.412	-1.444	1.00	92.62	D
3001	O	ASP	626	22.289	16.493	-1.655	1.00	92.92	D
3002	N	LEU	627	23.749	18.013	-2.436	1.00	91.17	D
3003	CA	LEU	627	23.584	17.593	-3.840	1.00	89.74	D
3004	CB	LEU	627	22.161	17.873	-4.367	1.00	88.17	D
3005	CG	LEU	627	21.783	17.274	-5.744	1.00	87.34	D
3006	CD1	LEU	627	20.342	17.608	-6.076	1.00	87.00	D
3007	CD2	LEU	627	22.674	17.807	-6.855	1.00	87.14	D
3008	C	LEU	627	24.587	18.216	-4.805	1.00	89.11	D
3009	O	LEU	627	24.358	19.297	-5.368	1.00	88.73	D
3010	N	ILE	628	25.674	17.476	-5.005	1.00	88.58	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
10	3011	CA	ILE	628	26.777	17.834	-5.882	1.00	87.30	D
	3012	CB	ILE	628	28.120	17.568	-5.204	1.00	86.84	D
	3013	CG2	ILE	628	29.256	17.957	-6.120	1.00	86.63	D
	3014	CG1	ILE	628	28.175	18.310	-3.873	1.00	86.64	D
	3015	CD1	ILE	628	29.556	18.369	-3.261	1.00	86.21	D
15	3016	C	ILE	628	26.743	16.966	-7.128	1.00	86.45	D
	3017	O	ILE	628	26.406	15.783	-7.074	1.00	85.46	D
20	3018	N	ILE	629	27.087	17.543	-8.264	1.00	86.29	D
	3019	CA	ILE	629	27.103	16.735	-9.443	1.00	86.10	D
	3020	CB	ILE	629	26.472	17.449	-10.621	1.00	84.49	D
	3021	CG2	ILE	629	27.090	16.998	-11.939	1.00	82.56	D
	3022	CG1	ILE	629	24.978	17.158	-10.572	1.00	83.17	D
25	3023	CD1	ILE	629	24.175	18.036	-11.424	1.00	84.20	D
	3024	C	ILE	629	28.527	16.352	-9.684	1.00	87.80	D
	3025	O	ILE	629	29.310	17.095	-10.275	1.00	87.90	D
30	3026	N	ASN	630	28.840	15.190	-9.129	1.00	90.07	D
	3027	CA	ASN	630	30.127	14.525	-9.210	1.00	91.27	D
	3028	CB	ASN	630	30.121	13.359	-8.248	1.00	90.47	D
	3029	CG	ASN	630	28.829	12.602	-8.339	1.00	90.42	D
35	3030	OD1	ASN	630	28.088	12.776	-9.314	1.00	90.62	D
	3031	ND2	ASN	630	28.536	11.777	-7.348	1.00	89.63	D
	3032	C	ASN	630	30.222	13.976	-10.627	1.00	92.33	D
40	3033	O	ASN	630	29.381	14.260	-11.495	1.00	91.85	D
	3034	N	GLU	631	31.228	13.141	-10.814	1.00	94.20	D
	3035	CA	GLU	631	31.525	12.554	-12.090	1.00	95.53	D
	3036	CB	GLU	631	32.843	11.896	-12.061	1.00	97.16	D
45	3037	CG	GLU	631	33.465	11.820	-13.378	1.00	99.89	D
	3038	CD	GLU	631	34.587	10.855	-13.290	1.00	101.71	D
	3039	OE1	GLU	631	35.675	11.248	-12.812	1.00	102.39	D
50	3040	OE2	GLU	631	34.359	9.683	-13.654	1.00	101.65	D
	3041	C	GLU	631	30.538	11.546	-12.304	1.00	95.35	D
	3042	O	GLU	631	29.768	11.682	-13.201	1.00	95.58	D
55	3043	N	GLN	632	30.609	10.478	-11.553	1.00	95.08	D
	3044	CA	GLN	632	29.542	9.588	-11.723	1.00	95.45	D
	3045	CB	GLN	632	29.154	9.224	-10.365	1.00	97.31	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3046	CG	GLN	632	28.446	8.037	-10.306	1.00	100.89	D
3047	CD	GLN	632	27.588	8.184	-9.158	1.00	103.01	D
3048	OE1	GLN	632	28.060	8.523	-8.072	1.00	103.65	D
3049	NE2	GLN	632	26.299	7.994	-9.362	1.00	103.97	D
3050	C	GLN	632	28.442	10.450	-12.433	1.00	94.61	D
3051	O	GLN	632	28.445	10.522	-13.637	1.00	95.69	D
3052	N	ARG	633	27.594	11.210	-11.729	1.00	92.32	D
3053	CA	ARG	633	26.507	11.993	-12.391	1.00	89.05	D
3054	CB	ARG	633	25.913	12.967	-11.405	1.00	87.98	D
3055	CG	ARG	633	25.233	12.225	-10.339	1.00	86.09	D
3056	CD	ARG	633	24.990	13.092	-9.180	1.00	84.99	D
3057	NE	ARG	633	24.176	12.385	-8.209	1.00	83.88	D
3058	CZ	ARG	633	23.971	12.830	-6.983	1.00	82.20	D
3059	NH1	ARG	633	24.530	13.968	-6.618	1.00	81.44	D
3060	NH2	ARG	633	23.217	12.146	-6.134	1.00	82.05	D
3061	C	ARG	633	26.688	12.732	-13.706	1.00	88.02	D
3062	O	ARG	633	25.868	12.640	-14.616	1.00	87.50	D
3063	N	MET	634	27.749	13.509	-13.764	1.00	86.51	D
3064	CA	MET	634	28.118	14.278	-14.926	1.00	85.73	D
3065	CB	MET	634	29.471	14.854	-14.672	1.00	85.01	D
3066	CG	MET	634	29.759	16.030	-15.488	1.00	85.81	D
3067	SD	MET	634	29.367	17.489	-14.539	1.00	85.72	D
3068	CE	MET	634	28.927	18.527	-15.819	1.00	85.08	D
3069	C	MET	634	28.259	13.421	-16.158	1.00	85.55	D
3070	O	MET	634	28.533	13.913	-17.241	1.00	84.84	D
3071	N	THR	635	28.101	12.127	-16.003	1.00	86.00	D
3072	CA	THR	635	28.322	11.281	-17.142	1.00	86.49	D
3073	CB	THR	635	28.999	10.036	-16.635	1.00	86.24	D
3074	OG1	THR	635	29.025	10.105	-15.217	1.00	88.35	D
3075	CG2	THR	635	30.436	10.000	-17.055	1.00	86.02	D
3076	C	THR	635	27.029	10.987	-17.878	1.00	86.60	D
3077	O	THR	635	27.055	10.407	-18.967	1.00	86.62	D
3078	N	LEU	636	25.935	11.501	-17.293	1.00	86.56	D
3079	CA	LEU	636	24.538	11.315	-17.714	1.00	86.65	D
3080	CB	LEU	636	23.580	11.669	-16.578	1.00	86.61	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3081	CG	LEU	636	23.837	10.975	-15.244	1.00	87.09	D
	3082	CD1	LEU	636	23.459	11.935	-14.143	1.00	87.05	D
10	3083	CD2	LEU	636	23.067	9.690	-15.100	1.00	86.70	D
	3084	C	LEU	636	23.950	11.908	-18.952	1.00	87.19	D
	3085	O	LEU	636	23.710	13.106	-19.057	1.00	86.40	D
15	3086	N	PRO	637	23.473	11.013	-19.798	1.00	88.07	D
	3087	CD	PRO	637	22.642	9.979	-19.135	1.00	88.43	D
	3088	CA	PRO	637	22.888	11.410	-21.067	1.00	89.09	D
	3089	CB	PRO	637	21.454	10.914	-20.970	1.00	89.17	D
20	3090	CG	PRO	637	21.539	9.716	-20.122	1.00	88.86	D
	3091	C	PRO	637	22.920	12.871	-21.475	1.00	89.60	D
	3092	O	PRO	637	23.318	13.197	-22.575	1.00	90.04	D
25	3093	N	CYS	638	22.562	13.798	-20.631	1.00	89.77	D
	3094	CA	CYS	638	22.496	15.085	-21.249	1.00	90.59	D
	3095	CB	CYS	638	21.027	15.318	-21.522	1.00	90.92	D
	3096	SG	CYS	638	20.576	15.454	-23.222	1.00	91.46	D
30	3097	C	CYS	638	23.031	16.160	-20.395	1.00	90.69	D
	3098	O	CYS	638	22.797	17.335	-20.639	1.00	91.18	D
	3099	N	MET	639	23.819	15.758	-19.429	1.00	90.76	D
35	3100	CA	MET	639	24.239	16.699	-18.451	1.00	90.74	D
	3101	CB	MET	639	24.472	15.923	-17.159	1.00	91.74	D
	3102	CG	MET	639	23.666	16.490	-16.026	1.00	92.82	D
	3103	SD	MET	639	22.527	15.549	-15.057	1.00	96.14	D
40	3104	CE	MET	639	23.011	16.324	-13.615	1.00	95.51	D
	3105	C	MET	639	25.365	17.641	-18.712	1.00	90.77	D
	3106	O	MET	639	25.222	18.866	-18.588	1.00	91.47	D
45	3107	N	TYR	640	26.493	17.061	-19.070	1.00	90.29	D
	3108	CA	TYR	640	27.665	17.840	-19.283	1.00	89.21	D
	3109	CB	TYR	640	28.749	16.976	-19.896	1.00	85.42	D
	3110	CG	TYR	640	30.015	17.737	-19.953	1.00	81.76	D
50	3111	CD1	TYR	640	30.667	18.086	-18.782	1.00	80.23	D
	3112	CE1	TYR	640	31.734	18.942	-18.800	1.00	79.42	D
	3113	CD2	TYR	640	30.474	18.254	-21.153	1.00	80.19	D
55	3114	CE2	TYR	640	31.544	19.112	-21.184	1.00	78.89	D
	3115	CZ	TYR	640	32.167	19.457	-20.002	1.00	78.88	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3116	OH	TYR	640	33.227	20.326	-20.008	1.00	78.74	D
3117	C	TYR	640	27.324	18.970	-20.202	1.00	90.99	D
3118	O	TYR	640	27.515	20.150	-19.900	1.00	91.28	D
3119	N	ASP	641	26.739	18.605	-21.313	1.00	92.71	D
3120	CA	ASP	641	26.447	19.619	-22.257	1.00	93.94	D
3121	CB	ASP	641	25.557	19.076	-23.309	1.00	97.46	D
3122	CG	ASP	641	25.977	19.569	-24.610	1.00	100.36	D
3123	OD1	ASP	641	26.403	20.747	-24.622	1.00	102.08	D
3124	OD2	ASP	641	25.917	18.810	-25.589	1.00	101.89	D
3125	C	ASP	641	25.902	20.934	-21.775	1.00	92.79	D
3126	O	ASP	641	26.134	21.979	-22.380	1.00	92.04	D
3127	N	GLN	642	25.203	20.886	-20.665	1.00	92.46	D
3128	CA	GLN	642	24.613	22.071	-20.127	1.00	92.28	D
3129	CB	GLN	642	23.176	21.768	-19.850	1.00	93.82	D
3130	CG	GLN	642	22.514	21.281	-21.065	1.00	97.01	D
3131	CD	GLN	642	21.906	22.436	-21.770	1.00	99.33	D
3132	OE1	GLN	642	21.991	23.566	-21.291	1.00	100.64	D
3133	NE2	GLN	642	21.251	22.175	-22.891	1.00	100.09	D
3134	C	GLN	642	25.269	22.435	-18.842	1.00	90.53	D
3135	O	GLN	642	25.014	23.495	-18.306	1.00	90.55	D
3136	N	CYS	643	26.110	21.576	-18.307	1.00	88.94	D
3137	CA	CYS	643	26.657	21.944	-17.011	1.00	88.17	D
3138	CB	CYS	643	26.827	20.735	-16.132	1.00	88.74	D
3139	SG	CYS	643	25.287	20.237	-15.425	1.00	91.87	D
3140	C	CYS	643	27.954	22.519	-17.224	1.00	86.91	D
3141	O	CYS	643	28.692	22.913	-16.323	1.00	86.37	D
3142	N	LYS	644	28.215	22.657	-18.472	1.00	85.71	D
3143	CA	LYS	644	29.502	23.050	-18.703	1.00	84.89	D
3144	CB	LYS	644	29.854	22.517	-20.028	1.00	86.51	D
3145	CG	LYS	644	29.634	23.541	-21.026	1.00	89.18	D
3146	CD	LYS	644	30.440	23.203	-22.199	1.00	91.39	D
3147	CE	LYS	644	29.585	22.496	-23.213	1.00	92.90	D
3148	NZ	LYS	644	30.446	21.988	-24.311	1.00	93.59	D
3149	C	LYS	644	29.645	24.519	-18.613	1.00	83.42	D
3150	O	LYS	644	30.699	25.003	-18.233	1.00	82.60	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3151	N	HIS	645	28.588	25.246	-18.936	1.00	81.98	D
	3152	CA	HIS	645	28.753	26.666	-18.883	1.00	80.20	D
10	3153	CB	HIS	645	27.705	27.352	-19.712	1.00	80.02	D
	3154	CG	HIS	645	27.935	27.162	-21.171	1.00	79.83	D
	3155	CD2	HIS	645	28.877	27.635	-21.990	1.00	79.20	D
15	3156	ND1	HIS	645	27.103	26.362	-21.947	1.00	79.63	D
	3157	CE1	HIS	645	27.551	26.380	-23.189	1.00	79.43	D
	3158	NE2	HIS	645	28.624	27.145	-23.247	1.00	79.34	D
	3159	C	HIS	645	28.752	27.168	-17.486	1.00	78.77	D
20	3160	O	HIS	645	29.191	28.277	-17.229	1.00	77.58	D
	3161	N	MET	646	28.283	26.332	-16.578	1.00	77.65	D
	3162	CA	MET	646	28.278	26.699	-15.176	1.00	76.48	D
25	3163	CB	MET	646	27.324	25.832	-14.421	1.00	78.58	D
	3164	CG	MET	646	25.939	26.304	-14.567	1.00	80.03	D
	3165	SD	MET	646	24.817	25.168	-13.806	1.00	84.57	D
	3166	CE	MET	646	24.055	24.523	-15.228	1.00	84.51	D
30	3167	C	MET	646	29.646	26.433	-14.645	1.00	74.60	D
	3168	O	MET	646	30.246	27.246	-13.946	1.00	74.05	D
	3169	N	LEU	647	30.099	25.230	-14.946	1.00	72.75	D
35	3170	CA	LEU	647	31.411	24.790	-14.567	1.00	71.39	D
	3171	CB	LEU	647	31.784	23.611	-15.428	1.00	71.41	D
	3172	CG	LEU	647	31.425	22.331	-14.726	1.00	71.96	D
	3173	CD1	LEU	647	31.553	21.158	-15.662	1.00	71.20	D
40	3174	CD2	LEU	647	32.354	22.209	-13.544	1.00	71.68	D
	3175	C	LEU	647	32.356	25.896	-14.896	1.00	70.66	D
	3176	O	LEU	647	33.367	26.131	-14.243	1.00	71.06	D
45	3177	N	TYR	648	32.001	26.580	-15.958	1.00	69.70	D
	3178	CA	TYR	648	32.823	27.626	-16.451	1.00	68.49	D
	3179	CB	TYR	648	32.243	28.113	-17.748	1.00	67.48	D
	3180	CG	TYR	648	32.924	29.359	-18.130	1.00	67.54	D
50	3181	CD1	TYR	648	34.227	29.323	-18.597	1.00	67.45	D
	3182	CE1	TYR	648	34.919	30.471	-18.849	1.00	68.42	D
	3183	CD2	TYR	648	32.311	30.589	-17.932	1.00	68.18	D
55	3184	CE2	TYR	648	32.987	31.753	-18.175	1.00	68.77	D
	3185	CZ	TYR	648	34.296	31.689	-18.646	1.00	70.60	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3186	OH	TYR	648	34.963	32.853	-18.948	1.00	72.77	D
3187	C	TYR	648	33.058	28.813	-15.535	1.00	68.18	D
3188	O	TYR	648	34.143	29.395	-15.524	1.00	68.25	D
3189	N	VAL	649	32.045	29.181	-14.776	1.00	67.31	D
3190	CA	VAL	649	32.165	30.349	-13.925	1.00	66.61	D
3191	CB	VAL	649	30.755	30.921	-13.625	1.00	65.52	D
3192	CG1	VAL	649	29.736	30.299	-14.581	1.00	63.01	D
3193	CG2	VAL	649	30.363	30.668	-12.194	1.00	64.50	D
3194	C	VAL	649	32.921	30.034	-12.642	1.00	67.05	D
3195	O	VAL	649	33.734	30.830	-12.167	1.00	66.32	D
3196	N	SER	650	32.631	28.856	-12.106	1.00	68.46	D
3197	CA	SER	650	33.239	28.336	-10.887	1.00	69.14	D
3198	CB	SER	650	32.687	26.951	-10.620	1.00	67.35	D
3199	OG	SER	650	33.743	26.091	-10.281	1.00	68.16	D
3200	C	SER	650	34.720	28.204	-11.135	1.00	70.15	D
3201	O	SER	650	35.566	28.269	-10.237	1.00	71.52	D
3202	N	SER	651	35.010	27.995	-12.402	1.00	69.47	D
3203	CA	SER	651	36.356	27.803	-12.836	1.00	68.31	D
3204	CB	SER	651	36.304	27.110	-14.181	1.00	69.50	D
3205	OG	SER	651	37.318	27.608	-15.023	1.00	70.83	D
3206	C	SER	651	37.086	29.121	-12.925	1.00	66.66	D
3207	O	SER	651	38.290	29.205	-12.729	1.00	65.24	D
3208	N	GLU	652	36.343	30.169	-13.216	1.00	66.35	D
3209	CA	GLU	652	36.957	31.461	-13.348	1.00	65.96	D
3210	CB	GLU	652	36.062	32.329	-14.197	1.00	66.68	D
3211	CG	GLU	652	36.131	31.903	-15.622	1.00	67.67	D
3212	CD	GLU	652	37.481	32.258	-16.202	1.00	69.84	D
3213	OE1	GLU	652	37.724	33.462	-16.411	1.00	70.18	D
3214	OE2	GLU	652	38.309	31.351	-16.428	1.00	72.00	D
3215	C	GLU	652	37.179	32.061	-11.996	1.00	64.92	D
3216	O	GLU	652	38.165	32.756	-11.753	1.00	63.63	D
3217	N	LEU	653	36.246	31.781	-11.109	1.00	65.42	D
3218	CA	LEU	653	36.338	32.277	-9.755	1.00	66.47	D
3219	CB	LEU	653	35.169	31.757	-8.957	1.00	66.41	D
3220	CG	LEU	653	33.934	32.597	-9.220	1.00	64.68	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3221	CD1	LEU	653	32.747	31.964	-8.559	1.00	62.94	D
	3222	CD2	LEU	653	34.178	33.993	-8.682	1.00	62.56	D
10	3223	C	LEU	653	37.602	31.727	-9.171	1.00	67.66	D
	3224	O	LEU	653	38.385	32.399	-8.511	1.00	67.27	D
	3225	N	HIS	654	37.780	30.457	-9.428	1.00	69.12	D
15	3226	CA	HIS	654	38.923	29.801	-8.923	1.00	70.49	D
	3227	CB	HIS	654	38.836	28.367	-9.293	1.00	74.35	D
	3228	CG	HIS	654	40.008	27.578	-8.800	1.00	78.11	D
	3229	CD2	HIS	654	41.218	27.362	-9.405	1.00	78.68	D
20	3230	ND1	HIS	654	40.019	26.988	-7.601	1.00	79.49	D
	3231	CE1	HIS	654	41.218	26.385	-7.421	1.00	80.11	D
	3232	NE2	HIS	654	41.924	26.610	-8.493	1.00	79.67	D
25	3233	C	HIS	654	40.182	30.367	-9.518	1.00	70.41	D
	3234	O	HIS	654	41.132	30.725	-8.821	1.00	71.08	D
	3235	N	ARG	655	40.202	30.409	-10.832	1.00	69.80	D
	3236	CA	ARG	655	41.370	30.896	-11.512	1.00	68.29	D
30	3237	CB	ARG	655	41.127	30.849	-13.002	1.00	68.53	D
	3238	CG	ARG	655	42.064	31.738	-13.755	1.00	67.31	D
	3239	CD	ARG	655	41.808	31.616	-15.211	1.00	67.45	D
35	3240	NE	ARG	655	40.945	32.665	-15.733	1.00	68.01	D
	3241	CZ	ARG	655	41.322	33.934	-15.833	1.00	69.26	D
	3242	NH1	ARG	655	42.533	34.286	-15.436	1.00	70.31	D
	3243	NH2	ARG	655	40.525	34.834	-16.396	1.00	70.41	D
40	3244	C	ARG	655	41.724	32.309	-11.109	1.00	67.75	D
	3245	O	ARG	655	42.889	32.670	-10.956	1.00	67.53	D
	3246	N	LEU	656	40.700	33.120	-10.945	1.00	67.39	D
45	3247	CA	LEU	656	40.917	34.501	-10.607	1.00	66.65	D
	3248	CB	LEU	656	39.739	35.301	-11.088	1.00	66.57	D
	3249	CG	LEU	656	40.126	36.495	-11.943	1.00	67.03	D
	3250	CD1	LEU	656	41.318	36.181	-12.810	1.00	65.91	D
50	3251	CD2	LEU	656	38.925	36.851	-12.783	1.00	66.92	D
	3252	C	LEU	656	41.099	34.703	-9.133	1.00	66.46	D
	3253	O	LEU	656	41.387	35.812	-8.677	1.00	64.34	D
55	3254	N	GLN	657	40.896	33.630	-8.380	1.00	66.91	D
	3255	CA	GLN	657	41.064	33.735	-6.958	1.00	67.19	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5									
10									
15									
20									
25									
30									
35									
40									
45									
50									
55									

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3291	CG	GLU	661	34.532	41.760	1.448	1.00	71.42	D
	3292	CD	GLU	661	35.342	42.747	2.256	1.00	74.29	D
10	3293	OE1	GLU	661	35.698	43.822	1.714	1.00	73.64	D
	3294	OE2	GLU	661	35.610	42.449	3.444	1.00	75.81	D
	3295	C	GLU	661	33.951	41.068	-2.186	1.00	66.87	D
15	3296	O	GLU	661	32.961	41.727	-2.508	1.00	67.41	D
	3297	N	GLU	662	34.868	40.688	-3.071	1.00	64.88	D
	3298	CA	GLU	662	34.686	41.042	-4.477	1.00	63.49	D
	3299	CB	GLU	662	35.873	40.599	-5.314	1.00	62.99	D
20	3300	CG	GLU	662	37.162	41.179	-4.843	1.00	64.63	D
	3301	CD	GLU	662	38.352	40.431	-5.382	1.00	65.77	D
	3302	OE1	GLU	662	38.304	39.176	-5.401	1.00	65.65	D
25	3303	OE2	GLU	662	39.334	41.096	-5.771	1.00	66.42	D
	3304	C	GLU	662	33.425	40.344	-4.991	1.00	62.59	D
	3305	O	GLU	662	32.602	40.943	-5.669	1.00	62.76	D
	3306	N	TYR	663	33.275	39.067	-4.666	1.00	61.55	D
30	3307	CA	TYR	663	32.116	38.296	-5.105	1.00	61.53	D
	3308	CB	TYR	663	32.173	36.903	-4.511	1.00	60.18	D
	3309	CG	TYR	663	30.842	36.207	-4.514	1.00	58.99	D
35	3310	CD1	TYR	663	30.358	35.603	-5.679	1.00	58.48	D
	3311	CE1	TYR	663	29.173	34.869	-5.674	1.00	57.76	D
	3312	CD2	TYR	663	30.098	36.076	-3.342	1.00	58.44	D
	3313	CE2	TYR	663	28.902	35.341	-3.324	1.00	58.34	D
40	3314	CZ	TYR	663	28.453	34.738	-4.497	1.00	57.94	D
	3315	OH	TYR	663	27.308	33.970	-4.496	1.00	57.87	D
	3316	C	TYR	663	30.767	38.908	-4.724	1.00	62.00	D
45	3317	O	TYR	663	29.829	38.924	-5.520	1.00	62.20	D
	3318	N	LEU	664	30.665	39.354	-3.481	1.00	62.05	D
	3319	CA	LEU	664	29.445	39.953	-2.986	1.00	61.47	D
	3320	CB	LEU	664	29.637	40.414	-1.538	1.00	59.38	D
50	3321	CG	LEU	664	29.465	39.343	-0.468	1.00	56.38	D
	3322	CD1	LEU	664	29.558	39.964	0.898	1.00	56.57	D
	3323	CD2	LEU	664	28.120	38.685	-0.643	1.00	54.70	D
55	3324	C	LEU	664	29.041	41.139	-3.858	1.00	61.76	D
	3325	O	LEU	664	27.897	41.235	-4.315	1.00	62.66	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3326	N	CYS	665	30.001	42.036	-4.062	1.00	60.92	D
3327	CA	CYS	665	29.814	43.223	-4.871	1.00	60.90	D
3328	CB	CYS	665	31.074	44.068	-4.861	1.00	61.24	D
3329	SG	CYS	665	31.426	44.837	-3.286	1.00	65.61	D
3330	C	CYS	665	29.496	42.865	-6.306	1.00	60.48	D
3331	O	CYS	665	28.707	43.530	-6.963	1.00	61.40	D
3332	N	MET	666	30.117	41.818	-6.803	1.00	60.26	D
3333	CA	MET	666	29.875	41.421	-8.171	1.00	61.32	D
3334	CB	MET	666	30.901	40.380	-8.603	1.00	62.78	D
3335	CG	MET	666	32.263	40.951	-8.889	1.00	64.66	D
3336	SD	MET	666	33.317	39.659	-9.479	1.00	66.42	D
3337	CE	MET	666	33.925	39.166	-8.028	1.00	65.54	D
3338	C	MET	666	28.473	40.873	-8.410	1.00	61.55	D
3339	O	MET	666	27.900	41.065	-9.487	1.00	61.02	D
3340	N	LYS	667	27.924	40.178	-7.419	1.00	61.13	D
3341	CA	LYS	667	26.595	39.607	-7.568	1.00	60.57	D
3342	CB	LYS	667	26.350	38.592	-6.466	1.00	59.74	D
3343	CG	LYS	667	25.239	37.616	-6.751	1.00	59.22	D
3344	CD	LYS	667	25.237	36.517	-5.690	1.00	60.32	D
3345	CE	LYS	667	24.654	36.991	-4.345	1.00	62.35	D
3346	NZ	LYS	667	25.373	38.129	-3.686	1.00	63.45	D
3347	C	LYS	667	25.547	40.710	-7.513	1.00	60.96	D
3348	O	LYS	667	24.472	40.594	-8.112	1.00	60.77	D
3349	N	THR	668	25.864	41.775	-6.782	1.00	60.79	D
3350	CA	THR	668	24.973	42.909	-6.658	1.00	60.41	D
3351	CB	THR	668	25.477	43.872	-5.594	1.00	61.34	D
3352	OG1	THR	668	25.395	43.225	-4.321	1.00	63.92	D
3353	CG2	THR	668	24.646	45.148	-5.575	1.00	61.41	D
3354	C	THR	668	24.996	43.561	-8.023	1.00	59.41	D
3355	O	THR	668	23.960	43.901	-8.568	1.00	59.47	D
3356	N	LEU	669	26.195	43.708	-8.580	1.00	58.91	D
3357	CA	LEU	669	26.346	44.279	-9.906	1.00	57.37	D
3358	CB	LEU	669	27.816	44.348	-10.293	1.00	55.15	D
3359	CG	LEU	669	28.451	45.738	-10.271	1.00	54.09	D
3360	CD1	LEU	669	27.548	46.728	-9.596	1.00	53.96	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3361	CD2	LEU	669	29.782	45.684	-9.566	1.00	54.12	D
	3362	C	LEU	669	25.577	43.457	-10.937	1.00	57.74	D
10	3363	O	LEU	669	25.001	44.015	-11.849	1.00	59.33	D
	3364	N	LEU	670	25.540	42.139	-10.809	1.00	57.67	D
	3365	CA	LEU	670	24.787	41.377	-11.803	1.00	58.56	D
15	3366	CB	LEU	670	24.977	39.878	-11.623	1.00	58.10	D
	3367	CG	LEU	670	26.318	39.252	-11.968	1.00	58.50	D
	3368	CD1	LEU	670	26.221	37.821	-11.498	1.00	57.91	D
	3369	CD2	LEU	670	26.640	39.314	-13.463	1.00	56.69	D
20	3370	C	LEU	670	23.296	41.656	-11.773	1.00	59.22	D
	3371	O	LEU	670	22.615	41.449	-12.768	1.00	59.43	D
	3372	N	LEU	671	22.786	42.095	-10.629	1.00	60.29	D
25	3373	CA	LEU	671	21.359	42.389	-10.500	1.00	59.73	D
	3374	CB	LEU	671	21.003	42.662	-9.035	1.00	57.31	D
	3375	CG	LEU	671	19.589	43.177	-8.782	1.00	55.23	D
	3376	CD1	LEU	671	18.578	42.139	-9.272	1.00	53.61	D
30	3377	CD2	LEU	671	19.409	43.482	-7.299	1.00	52.46	D
	3378	C	LEU	671	21.092	43.632	-11.334	1.00	60.95	D
	3379	O	LEU	671	20.006	43.804	-11.891	1.00	61.87	D
35	3380	N	LEU	672	22.117	44.476	-11.420	1.00	60.54	D
	3381	CA	LEU	672	22.058	45.718	-12.168	1.00	60.50	D
	3382	CB	LEU	672	22.810	46.795	-11.402	1.00	58.78	D
	3383	CG	LEU	672	22.413	46.856	-9.938	1.00	58.99	D
40	3384	CD1	LEU	672	23.175	47.964	-9.225	1.00	57.12	D
	3385	CD2	LEU	672	20.914	47.072	-9.865	1.00	58.80	D
	3386	C	LEU	672	22.726	45.538	-13.515	1.00	62.31	D
45	3387	O	LEU	672	23.130	46.520	-14.136	1.00	63.27	D
	3388	N	SER	673	22.826	44.295	-13.972	1.00	64.36	D
	3389	CA	SER	673	23.527	43.991	-15.217	1.00	67.18	D
	3390	CB	SER	673	24.130	42.588	-15.146	1.00	66.06	D
50	3391	OG	SER	673	23.144	41.590	-15.336	1.00	63.96	D
	3392	C	SER	673	22.840	44.150	-16.570	1.00	70.84	D
	3393	O	SER	673	23.468	43.919	-17.608	1.00	71.75	D
55	3394	N	SER	674	21.562	44.495	-16.587	1.00	73.68	D
	3395	CA	SER	674	20.911	44.726	-17.872	1.00	75.75	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3396	CB	SER	674	20.813	43.430	-18.723	1.00	74.70	D
3397	OG	SER	674	19.856	42.496	-18.265	1.00	74.10	D
3398	C	SER	674	19.570	45.403	-17.662	1.00	76.88	D
3399	O	SER	674	18.859	45.143	-16.694	1.00	76.90	D
3400	N	VAL	675	19.266	46.333	-18.554	1.00	79.18	D
3401	CA	VAL	675	18.034	47.082	-18.465	1.00	82.02	D
3402	CB	VAL	675	18.333	48.572	-18.122	1.00	81.32	D
3403	CG1	VAL	675	18.840	48.676	-16.689	1.00	80.99	D
3404	CG2	VAL	675	19.375	49.143	-19.084	1.00	81.53	D
3405	C	VAL	675	17.282	46.979	-19.783	1.00	84.34	D
3406	O	VAL	675	17.825	46.508	-20.788	1.00	84.33	D
3407	N	PRO	676	16.006	47.390	-19.792	1.00	86.71	D
3408	CD	PRO	676	15.247	48.061	-18.726	1.00	86.46	D
3409	CA	PRO	676	15.222	47.326	-21.019	1.00	89.31	D
3410	CB	PRO	676	13.828	47.717	-20.540	1.00	88.04	D
3411	CG	PRO	676	14.130	48.722	-19.485	1.00	86.61	D
3412	C	PRO	676	15.832	48.341	-21.978	1.00	92.02	D
3413	O	PRO	676	16.330	49.381	-21.537	1.00	92.35	D
3414	N	LYS	677	15.842	48.036	-23.272	1.00	94.90	D
3415	CA	LYS	677	16.407	48.972	-24.244	1.00	97.63	D
3416	CB	LYS	677	16.648	48.301	-25.598	1.00	98.89	D
3417	CG	LYS	677	16.682	49.263	-26.803	1.00	101.15	D
3418	CD	LYS	677	17.638	50.452	-26.628	1.00	103.43	D
3419	CE	LYS	677	17.643	51.363	-27.875	1.00	104.79	D
3420	NZ	LYS	677	18.011	50.655	-29.151	1.00	104.66	D
3421	C	LYS	677	15.422	50.100	-24.414	1.00	98.84	D
3422	O	LYS	677	14.555	50.055	-25.273	1.00	99.87	D
3423	N	ASP	678	15.573	51.114	-23.582	1.00	99.57	D
3424	CA	ASP	678	14.702	52.270	-23.583	1.00	100.29	D
3425	CB	ASP	678	13.225	51.869	-23.734	1.00	101.68	D
3426	CG	ASP	678	12.772	51.830	-25.198	1.00	103.54	D
3427	OD1	ASP	678	13.319	52.599	-26.020	1.00	103.41	D
3428	OD2	ASP	678	11.855	51.040	-25.518	1.00	104.45	D
3429	C	ASP	678	14.951	52.811	-22.196	1.00	100.06	D
3430	O	ASP	678	14.945	54.020	-21.966	1.00	100.74	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3431	N	GLY	679	15.194	51.884	-21.272	1.00	98.77	D
	3432	CA	GLY	679	15.483	52.273	-19.906	1.00	96.64	D
10	3433	C	GLY	679	14.346	52.099	-18.930	1.00	95.05	D
	3434	O	GLY	679	13.198	51.851	-19.309	1.00	95.43	D
	3435	N	LEU	680	14.677	52.258	-17.653	1.00	93.10	D
15	3436	CA	LEU	680	13.712	52.103	-16.580	1.00	91.98	D
	3437	CB	LEU	680	14.398	51.536	-15.332	1.00	91.95	D
	3438	CG	LEU	680	15.723	50.795	-15.513	1.00	91.77	D
	3439	CD1	LEU	680	16.303	50.412	-14.171	1.00	91.91	D
20	3440	CD2	LEU	680	15.494	49.569	-16.329	1.00	92.35	D
	3441	C	LEU	680	13.025	53.407	-16.199	1.00	90.95	D
	3442	O	LEU	680	13.467	54.493	-16.570	1.00	91.02	D
25	3443	N	LYS	681	11.943	53.271	-15.442	1.00	90.04	D
	3444	CA	LYS	681	11.173	54.410	-14.964	1.00	89.16	D
	3445	CB	LYS	681	9.975	53.931	-14.143	1.00	89.45	D
	3446	CG	LYS	681	8.980	53.086	-14.913	1.00	89.94	D
30	3447	CD	LYS	681	7.670	52.959	-14.154	1.00	90.41	D
	3448	CE	LYS	681	6.800	51.866	-14.745	1.00	91.27	D
	3449	NZ	LYS	681	5.491	51.754	-14.056	1.00	91.68	D
35	3450	C	LYS	681	12.050	55.290	-14.087	1.00	88.34	D
	3451	O	LYS	681	11.866	56.508	-14.019	1.00	88.29	D
	3452	N	SER	682	13.008	54.656	-13.419	1.00	87.39	D
	3453	CA	SER	682	13.913	55.358	-12.521	1.00	86.48	D
40	3454	CB	SER	682	13.803	54.761	-11.117	1.00	87.14	D
	3455	OG	SER	682	12.473	54.351	-10.838	1.00	87.46	D
	3456	C	SER	682	15.350	55.242	-13.012	1.00	85.57	D
45	3457	O	SER	682	16.278	55.196	-12.203	1.00	85.27	D
	3458	N	GLN	683	15.521	55.197	-14.330	1.00	84.91	D
	3459	CA	GLN	683	16.844	55.073	-14.948	1.00	84.23	D
	3460	CB	GLN	683	16.787	55.515	-16.413	1.00	83.77	D
50	3461	CG	GLN	683	18.108	55.393	-17.157	1.00	84.51	D
	3462	CD	GLN	683	18.644	53.969	-17.198	1.00	85.77	D
	3463	OE1	GLN	683	18.017	53.065	-17.766	1.00	85.99	D
55	3464	NE2	GLN	683	19.807	53.761	-16.595	1.00	85.67	D
	3465	C	GLN	683	17.853	55.924	-14.204	1.00	83.55	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3466	O	GLN	683	18.961	55.482	-13.894	1.00	83.89	D
3467	N	GLU	684	17.447	57.147	-13.921	1.00	83.39	D
3468	CA	GLU	684	18.256	58.112	-13.203	1.00	83.70	D
3469	CB	GLU	684	17.345	59.309	-12.795	1.00	86.45	D
3470	CG	GLU	684	15.864	58.957	-12.344	1.00	89.45	D
3471	CD	GLU	684	14.753	59.125	-13.432	1.00	91.23	D
3472	OE1	GLU	684	14.992	58.827	-14.626	1.00	91.14	D
3473	OE2	GLU	684	13.614	59.535	-13.077	1.00	91.97	D
3474	C	GLU	684	18.965	57.468	-11.988	1.00	82.04	D
3475	O	GLU	684	20.201	57.396	-11.931	1.00	81.53	D
3476	N	LEU	685	18.157	56.968	-11.057	1.00	80.84	D
3477	CA	LEU	685	18.585	56.321	-9.807	1.00	79.91	D
3478	CB	LEU	685	17.341	56.029	-8.964	1.00	79.23	D
3479	CG	LEU	685	17.327	56.378	-7.477	1.00	78.87	D
3480	CD1	LEU	685	16.478	55.346	-6.740	1.00	78.47	D
3481	CD2	LEU	685	18.742	56.376	-6.921	1.00	79.03	D
3482	C	LEU	685	19.368	55.013	-10.008	1.00	79.20	D
3483	O	LEU	685	20.294	54.682	-9.259	1.00	78.90	D
3484	N	PHE	686	18.950	54.256	-11.004	1.00	77.79	D
3485	CA	PHE	686	19.598	53.011	-11.333	1.00	76.60	D
3486	CB	PHE	686	19.024	52.503	-12.633	1.00	74.90	D
3487	CG	PHE	686	19.654	51.260	-13.106	1.00	73.91	D
3488	CD1	PHE	686	19.184	50.036	-12.669	1.00	73.55	D
3489	CD2	PHE	686	20.739	51.307	-13.969	1.00	73.72	D
3490	CE1	PHE	686	19.771	48.866	-13.091	1.00	73.58	D
3491	CE2	PHE	686	21.337	50.140	-14.405	1.00	74.95	D
3492	CZ	PHE	686	20.856	48.912	-13.959	1.00	74.68	D
3493	C	PHE	686	21.070	53.309	-11.528	1.00	76.92	D
3494	O	PHE	686	21.942	52.774	-10.845	1.00	76.88	D
3495	N	ASP	687	21.332	54.194	-12.481	1.00	77.62	D
3496	CA	ASP	687	22.687	54.562	-12.804	1.00	78.23	D
3497	CB	ASP	687	22.697	55.529	-13.983	1.00	79.48	D
3498	CG	ASP	687	22.345	54.836	-15.286	1.00	80.76	D
3499	OD1	ASP	687	22.659	53.632	-15.418	1.00	80.42	D
3500	OD2	ASP	687	21.768	55.489	-16.180	1.00	81.33	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GRα IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3501	C	ASP	687	23.420	55.140	-11.623	1.00	77.82	D
	3502	O	ASP	687	24.649	55.192	-11.610	1.00	77.25	D
10	3503	N	GLU	688	22.676	55.560	-10.614	1.00	77.40	D
	3504	CA	GLU	688	23.326	56.105	-9.444	1.00	77.00	D
	3505	CB	GLU	688	22.393	57.027	-8.699	1.00	79.26	D
15	3506	CG	GLU	688	23.115	57.790	-7.636	1.00	83.90	D
	3507	CD	GLU	688	22.167	58.405	-6.663	1.00	86.20	D
	3508	OE1	GLU	688	21.003	58.648	-7.061	1.00	87.82	D
	3509	OE2	GLU	688	22.587	58.648	-5.510	1.00	87.04	D
20	3510	C	GLU	688	23.724	54.954	-8.538	1.00	75.46	D
	3511	O	GLU	688	24.850	54.904	-8.027	1.00	75.05	D
	3512	N	ILE	689	22.789	54.032	-8.343	1.00	73.02	D
25	3513	CA	ILE	689	23.026	52.871	-7.514	1.00	70.61	D
	3514	CB	ILE	689	21.731	52.082	-7.351	1.00	71.16	D
	3515	CG2	ILE	689	21.977	50.724	-6.687	1.00	69.86	D
	3516	CG1	ILE	689	20.775	52.947	-6.542	1.00	71.37	D
30	3517	CD1	ILE	689	19.540	52.267	-6.190	1.00	72.58	D
	3518	C	ILE	689	24.092	52.043	-8.186	1.00	69.08	D
	3519	O	ILE	689	25.093	51.694	-7.572	1.00	68.64	D
35	3520	N	ARG	690	23.898	51.758	-9.463	1.00	67.58	D
	3521	CA	ARG	690	24.882	50.980	-10.186	1.00	67.61	D
	3522	CB	ARG	690	24.491	50.855	-11.644	1.00	65.92	D
	3523	CG	ARG	690	25.464	50.007	-12.435	1.00	65.20	D
40	3524	CD	ARG	690	24.717	49.473	-13.621	1.00	66.02	D
	3525	NE	ARG	690	25.445	48.547	-14.481	1.00	64.92	D
	3526	CZ	ARG	690	26.646	48.781	-14.997	1.00	65.68	D
45	3527	NH1	ARG	690	27.285	49.912	-14.727	1.00	65.29	D
	3528	NH2	ARG	690	27.179	47.904	-15.839	1.00	66.43	D
	3529	C	ARG	690	26.308	51.527	-10.117	1.00	68.89	D
	3530	O	ARG	690	27.264	50.756	-10.127	1.00	70.04	D
50	3531	N	MET	691	26.465	52.846	-10.065	1.00	70.17	D
	3532	CA	MET	691	27.795	53.438	-10.002	1.00	70.49	D
	3533	CB	MET	691	27.708	54.940	-10.291	1.00	73.73	D
55	3534	CG	MET	691	29.047	55.648	-10.500	1.00	77.42	D
	3535	SD	MET	691	29.970	54.941	-11.898	1.00	82.38	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3536	CE	MET	691	31.370	54.338	-11.036	1.00	81.52	D
3537	C	MET	691	28.418	53.205	-8.626	1.00	69.68	D
3538	O	MET	691	29.625	52.981	-8.506	1.00	68.71	D
3539	N	THR	692	27.579	53.256	-7.591	1.00	69.09	D
3540	CA	THR	692	28.033	53.068	-6.213	1.00	68.99	D
3541	CB	THR	692	26.918	53.278	-5.201	1.00	68.68	D
3542	OG1	THR	692	26.208	54.478	-5.503	1.00	68.25	D
3543	CG2	THR	692	27.518	53.382	-3.812	1.00	68.52	D
3544	C	THR	692	28.572	51.672	-5.977	1.00	69.04	D
3545	O	THR	692	29.567	51.491	-5.258	1.00	68.26	D
3546	N	TYR	693	27.901	50.672	-6.543	1.00	68.04	D
3547	CA	TYR	693	28.422	49.339	-6.376	1.00	67.90	D
3548	CB	TYR	693	27.340	48.267	-6.564	1.00	67.99	D
3549	CG	TYR	693	26.389	48.214	-5.384	1.00	68.55	D
3550	CD1	TYR	693	26.855	47.903	-4.103	1.00	67.96	D
3551	CE1	TYR	693	26.014	47.999	-2.991	1.00	68.49	D
3552	CD2	TYR	693	25.056	48.599	-5.523	1.00	67.38	D
3553	CE2	TYR	693	24.216	48.696	-4.424	1.00	67.56	D
3554	CZ	TYR	693	24.699	48.402	-3.160	1.00	68.22	D
3555	OH	TYR	693	23.879	48.568	-2.066	1.00	68.00	D
3556	C	TYR	693	29.597	49.128	-7.320	1.00	67.31	D
3557	O	TYR	693	30.340	48.184	-7.142	1.00	67.67	D
3558	N	ILE	694	29.810	49.978	-8.321	1.00	67.26	D
3559	CA	ILE	694	30.994	49.711	-9.133	1.00	68.01	D
3560	CB	ILE	694	30.998	50.412	-10.506	1.00	67.45	D
3561	CG2	ILE	694	32.387	50.264	-11.151	1.00	64.83	D
3562	CG1	ILE	694	29.964	49.750	-11.419	1.00	66.41	D
3563	CD1	ILE	694	29.460	50.643	-12.516	1.00	63.94	D
3564	C	ILE	694	32.218	50.151	-8.346	1.00	68.58	D
3565	O	ILE	694	33.273	49.533	-8.434	1.00	67.69	D
3566	N	LYS	695	32.073	51.216	-7.566	1.00	69.57	D
3567	CA	LYS	695	33.187	51.680	-6.755	1.00	70.84	D
3568	CB	LYS	695	32.959	53.124	-6.318	1.00	72.69	D
3569	CG	LYS	695	33.000	54.142	-7.451	1.00	74.90	D
3570	CD	LYS	695	32.390	55.440	-6.948	1.00	76.94	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3571	CE	LYS	695	32.702	56.654	-7.812	1.00	78.21	D
	3572	NZ	LYS	695	32.248	57.896	-7.098	1.00	78.41	D
10	3573	C	LYS	695	33.293	50.757	-5.539	1.00	70.27	D
	3574	O	LYS	695	34.367	50.579	-4.967	1.00	70.82	D
	3575	N	GLU	696	32.168	50.170	-5.155	1.00	69.31	D
15	3576	CA	GLU	696	32.146	49.253	-4.033	1.00	68.61	D
	3577	CB	GLU	696	30.702	48.845	-3.749	1.00	69.60	D
	3578	CG	GLU	696	30.362	48.549	-2.281	1.00	71.86	D
	3579	CD	GLU	696	31.072	49.454	-1.271	1.00	72.47	D
20	3580	OE1	GLU	696	30.972	50.702	-1.370	1.00	73.30	D
	3581	OE2	GLU	696	31.730	48.892	-0.364	1.00	72.64	D
	3582	C	GLU	696	32.998	48.053	-4.456	1.00	68.13	D
25	3583	O	GLU	696	33.702	47.452	-3.635	1.00	68.67	D
	3584	N	LEU	697	32.942	47.722	-5.747	1.00	66.69	D
	3585	CA	LEU	697	33.730	46.618	-6.278	1.00	64.43	D
	3586	CB	LEU	697	33.386	46.321	-7.745	1.00	61.53	D
30	3587	CG	LEU	697	34.306	45.230	-8.301	1.00	60.09	D
	3588	CD1	LEU	697	34.268	44.066	-7.340	1.00	58.33	D
	3589	CD2	LEU	697	33.902	44.789	-9.690	1.00	58.82	D
35	3590	C	LEU	697	35.165	47.078	-6.190	1.00	64.59	D
	3591	O	LEU	697	36.064	46.325	-5.824	1.00	65.27	D
	3592	N	GLY	698	35.363	48.345	-6.518	1.00	65.37	D
	3593	CA	GLY	698	36.689	48.930	-6.489	1.00	66.92	D
40	3594	C	GLY	698	37.407	48.840	-5.154	1.00	67.72	D
	3595	O	GLY	698	38.576	48.466	-5.112	1.00	66.59	D
	3596	N	LYS	699	36.716	49.198	-4.072	1.00	69.34	D
45	3597	CA	LYS	699	37.292	49.149	-2.725	1.00	70.05	D
	3598	CB	LYS	699	36.300	49.663	-1.706	1.00	70.00	D
	3599	CG	LYS	699	35.875	51.067	-1.896	1.00	71.97	D
	3600	CD	LYS	699	34.768	51.376	-0.924	1.00	72.69	D
50	3601	CE	LYS	699	34.729	52.853	-0.670	1.00	74.06	D
	3602	NZ	LYS	699	33.664	53.216	0.290	1.00	77.09	D
	3603	C	LYS	699	37.630	47.721	-2.332	1.00	71.03	D
55	3604	O	LYS	699	38.694	47.449	-1.771	1.00	70.60	D
	3605	N	ALA	700	36.690	46.819	-2.591	1.00	71.91	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3606	CA	ALA	700	36.875	45.422	-2.268	1.00	72.27	D
	3607	CB	ALA	700	35.713	44.601	-2.790	1.00	71.48	D
10	3608	C	ALA	700	38.171	45.004	-2.938	1.00	73.71	D
	3609	O	ALA	700	38.994	44.321	-2.333	1.00	73.83	D
	3610	N	ILE	701	38.351	45.434	-4.184	1.00	75.21	D
15	3611	CA	ILE	701	39.564	45.110	-4.927	1.00	77.37	D
	3612	CB	ILE	701	39.509	45.654	-6.370	1.00	76.34	D
	3613	CG2	ILE	701	40.884	45.535	-7.015	1.00	74.87	D
	3614	CG1	ILE	701	38.471	44.881	-7.185	1.00	76.01	D
20	3615	CD1	ILE	701	38.142	45.515	-8.531	1.00	75.37	D
	3616	C	ILE	701	40.832	45.656	-4.255	1.00	79.07	D
	3617	O	ILE	701	41.787	44.909	-4.047	1.00	79.07	D
25	3618	N	VAL	702	40.846	46.952	-3.919	1.00	81.82	D
	3619	CA	VAL	702	42.015	47.567	-3.280	1.00	84.95	D
	3620	CB	VAL	702	41.891	49.117	-3.042	1.00	83.97	D
	3621	CG1	VAL	702	41.611	49.843	-4.326	1.00	82.62	D
30	3622	CG2	VAL	702	40.838	49.409	-1.989	1.00	84.13	D
	3623	C	VAL	702	42.358	47.002	-1.914	1.00	87.59	D
	3624	O	VAL	702	43.524	46.983	-1.539	1.00	88.96	D
35	3625	N	LYS	703	41.356	46.562	-1.157	1.00	89.94	D
	3626	CA	LYS	703	41.632	46.050	0.176	1.00	93.02	D
	3627	CB	LYS	703	40.491	46.447	1.146	1.00	92.54	D
	3628	CG	LYS	703	39.544	45.321	1.640	1.00	92.88	D
40	3629	CD	LYS	703	38.695	45.782	2.857	1.00	93.01	D
	3630	CE	LYS	703	38.111	44.620	3.689	1.00	92.79	D
	3631	NZ	LYS	703	37.288	45.073	4.865	1.00	91.91	D
45	3632	C	LYS	703	41.898	44.549	0.243	1.00	95.67	D
	3633	O	LYS	703	41.770	43.948	1.301	1.00	96.69	D
	3634	N	ARG	704	42.300	43.942	-0.870	1.00	98.62	D
	3635	CA	ARG	704	42.564	42.501	-0.878	1.00	101.79	D
50	3636	CB	ARG	704	41.570	41.781	-1.805	1.00	101.22	D
	3637	CG	ARG	704	41.793	40.262	-1.931	1.00	102.41	D
	3638	CD	ARG	704	41.167	39.671	-3.209	1.00	102.72	D
55	3639	NE	ARG	704	42.151	39.345	-4.247	1.00	103.97	D
	3640	CZ	ARG	704	42.771	38.170	-4.365	1.00	104.85	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3641	NH1	ARG	704	42.519	37.190	-3.505	1.00	105.29	D
	3642	NH2	ARG	704	43.647	37.972	-5.346	1.00	104.19	D
10	3643	C	ARG	704	43.962	42.238	-1.396	1.00	104.43	D
	3644	O	ARG	704	44.690	41.370	-0.910	1.00	104.44	D
	3645	N	GLU	705	44.303	43.031	-2.403	1.00	107.72	D
15	3646	CA	GLU	705	45.556	42.951	-3.126	1.00	110.81	D
	3647	CB	GLU	705	45.508	43.963	-4.280	1.00	111.68	D
	3648	CG	GLU	705	45.679	43.371	-5.688	1.00	113.18	D
	3649	CD	GLU	705	44.861	42.108	-5.932	1.00	115.18	D
20	3650	OE1	GLU	705	43.628	42.131	-5.713	1.00	116.70	D
	3651	OE2	GLU	705	45.454	41.089	-6.355	1.00	116.07	D
	3652	C	GLU	705	46.853	43.097	-2.338	1.00	112.03	D
25	3653	O	GLU	705	47.368	42.128	-1.781	1.00	112.47	D
	3654	N	GLY	706	47.378	44.313	-2.286	1.00	113.33	D
	3655	CA	GLY	706	48.642	44.519	-1.616	1.00	115.12	D
	3656	C	GLY	706	49.598	44.812	-2.756	1.00	116.18	D
30	3657	O	GLY	706	50.261	43.918	-3.292	1.00	116.43	D
	3658	N	ASN	707	49.609	46.086	-3.131	1.00	116.60	D
	3659	CA	ASN	707	50.415	46.664	-4.208	1.00	116.29	D
35	3660	CB	ASN	707	50.762	45.618	-5.279	1.00	116.94	D
	3661	CG	ASN	707	52.236	45.209	-5.260	1.00	117.97	D
	3662	OD1	ASN	707	52.875	45.106	-6.312	1.00	118.42	D
	3663	ND2	ASN	707	52.775	44.960	-4.069	1.00	118.55	D
40	3664	C	ASN	707	49.514	47.771	-4.776	1.00	115.24	D
	3665	O	ASN	707	48.949	48.546	-4.003	1.00	115.85	D
	3666	N	SER	708	49.359	47.857	-6.093	1.00	113.05	D
45	3667	CA	SER	708	48.501	48.896	-6.666	1.00	111.02	D
	3668	CB	SER	708	48.887	50.285	-6.133	1.00	111.30	D
	3669	OG	SER	708	48.094	50.649	-5.015	1.00	110.98	D
	3670	C	SER	708	48.501	48.939	-8.184	1.00	109.52	D
50	3671	O	SER	708	47.654	49.603	-8.788	1.00	109.82	D
	3672	N	SER	709	49.454	48.266	-8.813	1.00	106.92	D
	3673	CA	SER	709	49.455	48.261	-10.267	1.00	104.39	D
55	3674	CB	SER	709	50.868	48.082	-10.827	1.00	104.45	D
	3675	OG	SER	709	51.334	46.758	-10.667	1.00	104.39	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3676	C	SER	709	48.564	47.098	-10.668	1.00	102.82	D
	3677	O	SER	709	47.962	47.094	-11.744	1.00	102.65	D
10	3678	N	GLN	710	48.465	46.108	-9.786	1.00	100.52	D
	3679	CA	GLN	710	47.622	44.966	-10.069	1.00	97.80	D
	3680	CB	GLN	710	48.159	43.697	-9.379	1.00	100.41	D
15	3681	CG	GLN	710	48.133	43.680	-7.855	1.00	104.43	D
	3682	CD	GLN	710	48.672	44.953	-7.233	1.00	106.82	D
	3683	OE1	GLN	710	49.775	45.397	-7.559	1.00	108.23	D
	3684	NE2	GLN	710	47.898	45.543	-6.329	1.00	108.12	D
20	3685	C	GLN	710	46.203	45.298	-9.622	1.00	94.01	D
	3686	O	GLN	710	45.322	44.442	-9.640	1.00	93.94	D
	3687	N	ASN	711	45.978	46.553	-9.240	1.00	89.32	D
25	3688	CA	ASN	711	44.640	46.949	-8.823	1.00	84.80	D
	3689	CB	ASN	711	44.688	48.108	-7.839	1.00	84.11	D
	3690	CG	ASN	711	44.719	47.619	-6.411	1.00	84.22	D
	3691	OD1	ASN	711	44.669	48.406	-5.474	1.00	84.93	D
30	3692	ND2	ASN	711	44.802	46.301	-6.237	1.00	83.76	D
	3693	C	ASN	711 1	43.714	47.252	-9.981	1.00	81.96	D
	3694	O	ASN	711	42.601	46.735	-10.017	1.00	81.02	D
35	3695	N	TRP	712	44.139	48.079	-10.930	1.00	78.84	D
	3696	CA	TRP	712	43.273	48.298	-12.073	1.00	75.28	D
	3697	CB	TRP	712	43.780	49.379	-12.988	1.00	74.46	D
	3698	CG	TRP	712	43.507	50.684	-12.489	1.00	73.88	D
40	3699	CD2	TRP	712	42.538	51.601	-12.996	1.00	74.08	D
	3700	CE2	TRP	712	42.647	52.778	-12.231	1.00	73.76	D
	3701	CE3	TRP	712	41.587	51.548	-14.032	1.00	74.01	D
45	3702	CD1	TRP	712	44.137	51.304	-11.464	1.00	73.42	D
	3703	NE1	TRP	712	43.631	52.565	-11.297	1.00	73.37	D
	3704	CZ2	TRP	712	41.841	53.901	-12.456	1.00	73.06	D
	3705	CZ3	TRP	712	40.780	52.663	-14.258	1.00	72.71	D
50	3706	CH2	TRP	712	40.918	53.828	-13.474	1.00	72.39	D
	3707	C	TRP	712	43.287	47.025	-12.863	1.00	74.11	D
	3708	O	TRP	712	42.325	46.687	-13.535	1.00	74.07	D
55	3709	N	GLN	713	44.388	46.304	-12.817	1.00	72.50	D
	3710	CA	GLN	713	44.379	45.095	-13.582	1.00	71.13	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3711	CB	GLN	713	45.753	44.459	-13.606	1.00	72.88	D
	3712	CG	GLN	713	45.816	43.299	-14.564	1.00	73.89	D
10	3713	CD	GLN	713	47.108	42.544	-14.428	1.00	75.34	D
	3714	OE1	GLN	713	47.438	41.708	-15.269	1.00	76.79	D
	3715	NE2	GLN	713	47.847	42.826	-13.359	1.00	75.96	D
15	3716	C	GLN	713	43.349	44.128	-13.016	1.00	69.75	D
	3717	O	GLN	713	42.760	43.357	-13.764	1.00	69.68	D
	3718	N	ARG	714	43.125	44.181	-11.701	1.00	68.00	D
	3719	CA	ARG	714	42.162	43.294	-11.021	1.00	66.56	D
20	3720	CB	ARG	714	42.267	43.521	-9.508	1.00	66.48	D
	3721	CG	ARG	714	41.495	42.575	-8.623	1.00	64.93	D
	3722	CD	ARG	714	42.015	41.157	-8.695	1.00	64.89	D
25	3723	NE	ARG	714	41.283	40.327	-7.752	1.00	64.24	D
	3724	CZ	ARG	714	41.209	39.007	-7.806	1.00	64.10	D
	3725	NH1	ARG	714	41.824	38.344	-8.770	1.00	63.98	D
	3726	NH2	ARG	714	40.496	38.351	-6.906	1.00	64.35	D
30	3727	C	ARG	714	40.757	43.636	-11.510	1.00	65.72	D
	3728	O	ARG	714	40.010	42.788	-12.009	1.00	64.06	D
	3729	N	PHE	715	40.422	44.905	-11.342	1.00	65.51	D
35	3730	CA	PHE	715	39.158	45.457	-11.757	1.00	66.56	D
	3731	CB	PHE	715	39.241	46.968	-11.699	1.00	65.63	D
	3732	CG	PHE	715	37.954	47.644	-11.950	1.00	66.28	D
	3733	CD1	PHE	715	36.831	47.302	-11.209	1.00	67.11	D
40	3734	CD2	PHE	715	37.858	48.655	-12.890	1.00	66.76	D
	3735	CE1	PHE	715	35.629	47.956	-11.397	1.00	66.49	D
	3736	CE2	PHE	715	36.650	49.324	-13.090	1.00	66.75	D
45	3737	CZ	PHE	715	35.535	48.974	-12.339	1.00	66.22	D
	3738	C	PHE	715	38.876	45.034	-13.182	1.00	67.61	D
	3739	O	PHE	715	37.832	44.448	-13.488	1.00	69.43	D
	3740	N	TYR	716	39.818	45.349	-14.056	1.00	67.76	D
50	3741	CA	TYR	716	39.691	45.012	-15.452	1.00	67.50	D
	3742	CB	TYR	716	40.993	45.341	-16.172	1.00	68.51	D
	3743	CG	TYR	716	40.999	44.951	-17.618	1.00	69.44	D
55	3744	CD1	TYR	716	40.438	45.773	-18.594	1.00	69.90	D
	3745	CE1	TYR	716	40.411 1	45.381	-19.929	1.00	71.02	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3746	CD2	TYR	716	41.538	43.733	-18.006	1.00	70.06	D
3747	CE2	TYR	716	41.516	43.332	-19.321	1.00	71.47	D
3748	CZ	TYR	716	40.953	44.155	-20.282	1.00	71.73	D
3749	OH	TYR	716	40.934	43.726	-21.590	1.00	73.37	D
3750	C	TYR	716	39.327	43.532	-15.592	1.00	67.55	D
3751	O	TYR	716	38.400	43.191	-16.321	1.00	68.03	D
3752	N	GLN	717	40.020	42.655	-14.879	1.00	67.25	D
3753	CA	GLN	717	39.711	41.230	-14.973	1.00	68.01	D
3754	CB	GLN	717	40.794	40.384	-14.327	1.00	69.66	D
3755	CG	GLN	717	42.189	40.709	-14.740	1.00	72.77	D
3756	CD	GLN	717	43.173	39.799	-14.052	1.00	75.40	D
3757	OE1	GLN	717	43.559	40.028	-12.899	1.00	76.60	D
3758	NE2	GLN	717	43.566	38.738	-14.744	1.00	76.67	D
3759	C	GLN	717	38.387	40.863	-14.307	1.00	67.82	D
3760	O	GLN	717	37.608	40.067	-14.848	1.00	67.36	D
3761	N	LEU	718	38.132	41.405	-13.120	1.00	66.52	D
3762	CA	LEU	718	36.879	41.066	-12.470	1.00	64.77	D
3763	CB	LEU	718	36.784	41.711	-11.078	1.00	62.27	D
3764	CG	LEU	718	37.739	41.100	-10.040	1.00	60.26	D
3765	CD1	LEU	718	37.496	41.700	-8.674	1.00	58.48	D
3766	CD2	LEU	718	37.529	39.596	-9.976	1.00	60.78	D
3767	C	LEU	718	35.731	41.493	-13.390	1.00	64.36	D
3768	O	LEU	718	34.859	40.686	-13.713	1.00	63.38	D
3769	N	THR	719	35.760	42.740	-13.855	1.00	64.39	D
3770	CA	THR	719	34.704	43.227	-14.738	1.00	65.59	D
3771	CB	THR	719	34.833	44.729	-14.972	1.00	64.69	D
3772	OG1	THR	719	36.133	45.020	-15.505	1.00	63.56	D
3773	CG2	THR	719	34.637	45.477	-13.660	1.00	64.71	D
3774	C	THR	719	34.648	42.507	-16.090	1.00	66.44	D
3775	O	THR	719	33.690	42.674	-16.853	1.00	66.27	D
3776	N	LYS	720	35.666	41.709	-16.396	1.00	67.02	D
3777	CA	LYS	720	35.650	40.980	-17.654	1.00	66.94	D
3778	CB	LYS	720	37.048	40.497	-18.036	1.00	69.93	D
3779	CG	LYS	720	37.235	40.307	-19.547	1.00	74.14	D
3780	CD	LYS	720	37.418	41.656	-20.262	1.00	77.44	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3781	CE	LYS	720	37.399	41.534	-21.799	1.00	79.51	D
	3782	NZ	LYS	720	37.765	42.813	-22.503	1.00	80.62	D
10	3783	C	LYS	720	34.741	39.789	-17.405	1.00	65.29	D
	3784	O	LYS	720	33.925	39.420	-18.247	1.00	65.38	D
	3785	N	LEU	721	34.881	39.207	-16.218	1.00	63.82	D
15	3786	CA	LEU	721	34.073	38.068	-15.818	1.00	62.57	D
	3787	CB	LEU	721	34.473	37.616	-14.420	1.00	60.12	D
	3788	CG	LEU	721	34.373	36.116	-14.199	1.00	60.11	D
	3789	CD1	LEU	721	34.104	35.890	-12.732	1.00	59.49	D
20	3790	CD2	LEU	721	33.261	35.499	-15.051	1.00	59.33	D
	3791	C	LEU	721	32.596	38.467	-15.823	1.00	62.94	D
	3792	O	LEU	721	31.732	37.701	-16.263	1.00	63.51	D
25	3793	N	LEU	722	32.315	39.666	-15.324	1.00	62.68	D
	3794	CA	LEU	722	30.951	40.170	-15.287	1.00	62.47	D
	3795	CB	LEU	722	30.926	41.583	-14.698	1.00	61.57	D
	3796	CG	LEU	722	31.240	41.519	-13.203	1.00	60.98	D
30	3797	CD1	LEU	722	31.132	42.877	-12.563	1.00	59.96	D
	3798	CD2	LEU	722	30.267	40.535	-12.553	1.00	59.00	D
	3799	C	LEU	722	30.347	40.167	-16.675	1.00	63.61	D
35	3800	O	LEU	722	29.330	39.525	-16.898	1.00	64.24	D
	3801	N	ASP	723	30.983	40.866	-17.609	1.00	63.93	D
	3802	CA	ASP	723	30.493	40.952	-18.983	1.00	63.89	D
	3803	CB	ASP	723	31.462	41.748	-19.844	1.00	64.74	D
40	3804	CG	ASP	723	31.485	43.200	-19.481	1.00	66.67	D
	3805	OD1	ASP	723	30.530	43.657	-18.817	1.00	68.28	D
	3806	OD2	ASP	723	32.445	43.890	-19.868	1.00	65.20	D
45	3807	C	ASP	723	30.280	39.608	-19.652	1.00	64.20	D
	3808	O	ASP	723	29.408	39.456	-20.509	1.00	63.99	D
	3809	N	SER	724	31.089	38.635	-19.263	1.00	64.29	D
	3810	CA	SER	724	31.009	37.311	-19.855	1.00	64.18	D
50	3811	CB	SER	724	32.353	36.610	-19.706	1.00	64.03	D
	3812	OG	SER	724	32.261	35.556	-18.769	1.00	65.88	D
	3813	C	SER	724	29.912	36.478	-19.218	1.00	63.99	D
55	3814	O	SER	724	29.685	35.322	-19.585	1.00	63.80	D
	3815	N	MET	725	29.234	37.086	-18.256	1.00	63.58	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3816	CA	MET	725	28.157	36.433	-17.533	1.00	62.50	D
3817	CB	MET	725	27.944	37.184	-16.225	1.00	60.73	D
3818	CG	MET	725	27.507	36.347	-15.077	1.00	59.86	D
3819	SD	MET	725	28.599	34.988	-14.747	1.00	57.82	D
3820	CE	MET	725	27.340	33.823	-14.381	1.00	56.09	D
3821	C	MET	725	26.911	36.479	-18.410	1.00	62.36	D
3822	O	MET	725	26.014	35.645	-18.289	1.00	61.95	D
3823	N	HIS	726	26.867	37.474	-19.294	1.00	62.70	D
3824	CA	HIS	726	25.754	37.598	-20.213	1.00	63.08	D
3825	CB	HIS	726	25.856	38.883	-21.038	1.00	60.89	D
3826	CG	HIS	726	25.427	40.114	-20.295	1.00	59.03	D
3827	CD2	HIS	726	24.277	40.399	-19.634	1.00	58.37	D
3828	ND1	HIS	726	26.228	41.224	-20.171	1.00	58.24	D
3829	CE1	HIS	726	25.595	42.144	-19.460	1.00	57.37	D
3830	NE2	HIS	726	24.413	41.669	-19.126	1.00	58.49	D
3831	C	HIS	726	25.850	36.383	-21.115	1.00	64.70	D
3832	O	HIS	726	24.873	35.676	-21.303	1.00	65.01	D
3833	N	GLU	727	27.031	36.091	-21.641	1.00	67.88	D
3834	CA	GLU	727	27.092	34.931	-22.504	1.00	70.51	D
3835	CB	GLU	727	28.390	34.864	-23.293	1.00	72.69	D
3836	CG	GLU	727	28.196	34.036	-24.552	1.00	77.47	D
3837	CD	GLU	727	29.485	33.473	-25.082	1.00	82.02	D
3838	OE1	GLU	727	30.495	34.219	-25.072	1.00	84.51	D
3839	OE2	GLU	727	29.483	32.291	-25.512	1.00	83.29	D
3840	C	GLU	727	26.842	33.585	-21.825	1.00	71.14	D
3841	O	GLU	727	26.305	32.685	-22.477	1.00	71.67	D
3842	N	VAL	728	27.211	33.395	-20.557	1.00	71.39	D
3843	CA	VAL	728	26.890	32.080	-19.992	1.00	71.03	D
3844	CB	VAL	728	27.794	31.638	-18.750	1.00	70.84	D
3845	CG1	VAL	728	28.705	32.749	-18.298	1.00	70.06	D
3846	CG2	VAL	728	26.921	31.121	-17.609	1.00	69.97	D
3847	C	VAL	728	25.397	32.019	-19.657	1.00	70.61	D
3848	O	VAL	728	24.783	30.964	-19.800	1.00	70.41	D
3849	N	VAL	729	24.806	33.146	-19.252	1.00	71.03	D
3850	CA	VAL	729	23.368	33.165	-18.948	1.00	72.03	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3851	CB	VAL	729	22.929	34.527	-18.317	1.00	72.41	D
	3852	CG1	VAL	729	21.547	34.949	-18.822	1.00	72.84	D
10	3853	CG2	VAL	729	22.873	34.382	-16.811	1.00	72.63	D
	3854	C	VAL	729	22.560	32.872	-20.216	1.00	72.63	D
	3855	O	VAL	729	21.558	32.166	-20.173	1.00	72.16	D
15	3856	N	GLU	730	22.996	33.403	-21.351	1.00	74.69	D
	3857	CA	GLU	730	22.289	33.131	-22.592	1.00	77.21	D
	3858	CB	GLU	730	23.013	33.756	-23.783	1.00	78.90	D
	3859	CG	GLU	730	22.218	33.663	-25.068	1.00	83.32	D
20	3860	CD	GLU	730	22.836	34.458	-26.198	1.00	86.77	D
	3861	OE1	GLU	730	23.326	35.580	-25.931	1.00	88.49	D
	3862	OE2	GLU	730	22.811	33.962	-27.351	1.00	88.56	D
25	3863	C	GLU	730	22.195	31.610	-22.771	1.00	77.66	D
	3864	O	GLU	730	21.104	31.057	-22.852	1.00	77.32	D
	3865	N	ASN	731	23.342	30.934	-22.801	1.00	78.69	D
	3866	CA	ASN	731	23.362	29.482	-22.972	1.00	79.39	D
30	3867	CB	ASN	731	24.808	29.046	-23.172	1.00	80.51	D
	3868	CG	ASN	731	25.367	29.753	-24.340	1.00	81.74	D
	3869	OD1	ASN	731	26.524	29.646	-24.728	1.00	83.00	D
35	3870	ND2	ASN	731	24.483	30.534	-24.946	1.00	84.04	D
	3871	C	ASN	731	22.649	28.770	-21.864	1.00	79.09	D
	3872	O	ASN	731	22.147	27.659	-22.040	1.00	78.14	D
40	3873	N	LEU	732	22.550	29.441	-20.731	1.00	79.35	D
	3874	CA	LEU	732	21.838	28.846	-19.639	1.00	79.99	D
	3875	CB	LEU	732	22.253	29.475	-18.331	1.00	78.02	D
	3876	CG	LEU	732	23.448	28.662	-17.877	1.00	76.80	D
45	3877	CD1	LEU	732	23.803	29.107	-16.496	1.00	76.83	D
	3878	CD2	LEU	732	23.124	27.158	-17.905	1.00	76.26	D
	3879	C	LEU	732	20.349	28.977	-19.856	1.00	81.89	D
	3880	O	LEU	732	19.600	28.065	-19.510	1.00	83.06	D
50	3881	N	LEU	733	19.913	30.090	-20.442	1.00	83.07	D
	3882	CA	LEU	733	18.487	30.283	-20.705	1.00	83.87	D
	3883	CB	LEU	733	18.172	31.759	-20.959	1.00	82.93	D
55	3884	CG	LEU	733	18.209	32.702	-19.752	1.00	82.42	D
	3885	CD1	LEU	733	18.026	34.120	-20.244	1.00	81.62	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3886	CD2	LEU	733	17.132	32.332	-18.738	1.00	81.48	D
3887	C	LEU	733	17.976	29.439	-21.873	1.00	85.02	D
3888	O	LEU	733	16.902	28.843	-21.764	1.00	84.76	D
3889	N	ASN	734	18.718	29.374	-22.979	1.00	86.42	D
3890	CA	ASN	734	18.259	28.555	-24.100	1.00	88.57	D
3891	CB	ASN	734	19.306	28.424	-25.236	1.00	88.99	D
3892	CG	ASN	734	19.540	29.733	-26.048	1.00	90.34	D
3893	OD1	ASN	734	18.745	30.685	-26.026	1.00	89.17	D
3894	ND2	ASN	734	20.652	29.748	-26.793	1.00	91.10	D
3895	C	ASN	734	17.838	27.123	-23.646	1.00	90.13	D
3896	O	ASN	734	16.761	26.706	-24.049	1.00	90.87	D
3897	N	TYR	735	18.631	26.380	-22.837	1.00	91.96	D
3898	CA	TYR	735	18.235	24.990	-22.412	1.00	93.75	D
3899	CB	TYR	735	19.265	24.176	-21.528	1.00	96.29	D
3900	CG	TYR	735	19.019	22.640	-21.651	1.00	99.41	D
3901	CD1	TYR	735	19.517	21.657	-20.741	1.00	101.17	D
3902	CE1	TYR	735	19.286	20.262	-20.977	1.00	102.99	D
3903	CD2	TYR	735	18.300	22.187	-22.738	1.00	100.65	D
3904	CE2	TYR	735	18.064	20.851	-22.963	1.00	101.77	D
3905	CZ	TYR	735	18.540	19.893	-22.097	1.00	103.45	D
3906	OH	TYR	735	18.225	18.584	-22.388	1.00	104.95	D
3907	C	TYR	735	17.015	25.084	-21.563	1.00	93.60	D
3908	O	TYR	735	16.179	24.194	-21.555	1.00	94.18	D
3909	N	CYS	736	16.907	26.177	-20.843	1.00	92.87	D
3910	CA	CYS	736	15.803	26.297	-19.942	1.00	92.13	D
3911	CB	CYS	736	16.125	27.357	-18.909	1.00	91.98	D
3912	SG	CYS	736	14.842	27.599	-17.686	1.00	92.43	D
3913	C	CYS	736	14.489	26.567	-20.621	1.00	91.67	D
3914	O	CYS	736	13.510	25.862	-20.381	1.00	91.52	D
3915	N	PHE	737	14.457	27.583	-21.468	1.00	91.07	D
3916	CA	PHE	737	13.220	27.872	-22.154	1.00	91.08	D
3917	CB	PHE	737	13.420	29.045	-23.104	1.00	89.07	D
3918	CG	PHE	737	13.666	30.364	-22.404	1.00	87.03	D
3919	CD1	PHE	737	13.388	30.521	-21.044	1.00	85.41	D
3920	CD2	PHE	737	14.114	31.465	-23.125	1.00	86.11	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3921	CE1	PHE	737	13.544	31.759	-20.422	1.00	84.26	D
	3922	CE2	PHE	737	14.274	32.706	-22.512	1.00	84.63	D
10	3923	CZ	PHE	737	13.991	32.854	-21.158	1.00	83.57	D
	3924	C	PHE	737	12.821	26.598	-22.896	1.00	92.41	D
	3925	O	PHE	737	11.734	26.054	-22.685	1.00	92.34	D
15	3926	N	GLN	738	13.730	26.120	-23.740	1.00	93.76	D
	3927	CA	GLN	738	13.534	24.904	-24.514	1.00	95.09	D
	3928	CB	GLN	738	14.888	24.425	-25.027	1.00	96.20	D
	3929	CG	GLN	738	14.873	23.403	-26.136	1.00	97.39	D
20	3930	CD	GLN	738	16.275	23.176	-26.656	1.00	98.13	D
	3931	OE1	GLN	738	17.001	22.299	-26.178	1.00	98.35	D
	3932	NE2	GLN	738	16.680	23.997	-27.621	1.00	98.37	D
25	3933	C	GLN	738	12.922	23.873	-23.585	1.00	95.89	D
	3934	O	GLN	738	11.711	23.743	-23.530	1.00	96.25	D
	3935	N	THR	739	13.750	23.155	-22.837	1.00	97.17	D
	3936	CA	THR	739	13.224	22.160	-21.915	1.00	98.69	D
30	3937	CB	THR	739	14.197	21.930	-20.764	1.00	98.17	D
	3938	OG1	THR	739	14.904	23.141	-20.495	1.00	98.69	D
	3939	CG2	THR	739	15.193	20.839	-21.115	1.00	98.02	D
35	3940	C	THR	739	11.831	22.533	-21.369	1.00	100.03	D
	3941	O	THR	739	10.915	21.708	-21.389	1.00	100.63	D
	3942	N	PHE	740	11.654	23.771	-20.921	1.00	101.15	D
	3943	CA	PHE	740	10.358	24.205	-20.388	1.00	102.20	D
40	3944	CB	PHE	740	10.470	25.629	-19.856	1.00	100.56	D
	3945	CG	PHE	740	9.179	26.181	-19.325	1.00	98.93	D
	3946	CD1	PHE	740	8.824	26.007	-17.994	1.00	98.31	D
45	3947	CD2	PHE	740	8.327	26.901	-20.152	1.00	97.96	D
	3948	CE1	PHE	740	7.647	26.542	-17.487	1.00	97.83	D
	3949	CE2	PHE	740	7.148	27.440	-19.658	1.00	97.24	D
	3950	CZ	PHE	740	6.806	27.263	-18.320	1.00	97.30	D
50	3951	C	PHE	740	9.197	24.140	-21.385	1.00	104.02	D
	3952	O	PHE	740	8.043	23.978	-20.987	1.00	103.68	D
	3953	N	LEU	741	9.495	24.291	-22.671	1.00	106.46	D
55	3954	CA	LEU	741	8.459	24.238	-23.696	1.00	109.10	D
	3955	CB	LEU	741	8.630	25.383	-24.699	1.00	108.94	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	3956	CG	LEU	741	8.799	26.819	-24.195	1.00	108.65	D
	3957	CD1	LEU	741	8.890	27.741	-25.405	1.00	108.53	D
10	3958	CD2	LEU	741	7.642	27.233	-23.299	1.00	108.26	D
	3959	C	LEU	741	8.493	22.901	-24.436	1.00	111.39	D
	3960	O	LEU	741	8.385	22.853	-25.666	1.00	111.44	D
15	3961	N	ASP	742	8.663	21.821	-23.676	1.00	114.02	D
	3962	CA	ASP	742	8.684	20.465	-24.222	1.00	116.52	D
	3963	CB	ASP	742	10.064	20.088	-24.764	1.00	117.48	D
	3964	CG	ASP	742	10.055	18.732	-25.451	1.00	119.20	D
20	3965	OD1	ASP	742	11.132	18.125	-25.638	1.00	119.74	D
	3966	OD2	ASP	742	8.949	18.278	-25.818	1.00	120.17	D
	3967	C	ASP	742	8.329	19.488	-23.115	1.00	117.76	D
25	3968	O	ASP	742	9.193	19.111	-22.319	1.00	117.68	D
	3969	N	LYS	743	7.073	19.060	-23.048	1.00	119.41	D
	3970	CA	LYS	743	6.746	18.138	-21.985	1.00	120.92	D
	3971	CB	LYS	743	5.381	18.418	-21.393	1.00	121.59	D
30	3972	CG	LYS	743	5.537	18.534	-19.898	1.00	122.24	D
	3973	CD	LYS	743	4.242	18.414	-19.164	1.00	122.77	D
	3974	CE	LYS	743	3.312	19.572	-19.487	1.00	122.90	D
35	3975	NZ	LYS	743	3.995	20.761	-20.080	1.00	122.44	D
	3976	C	LYS	743	6.885	16.671	-22.315	1.00	121.35	D
	3977	O	LYS	743	6.565	15.808	-21.495	1.00	121.83	D
	3978	N	THR	744	7.360	16.393	-23.523	1.00	121.55	D
40	3979	CA	THR	744	7.625	15.018	-23.914	1.00	121.69	D
	3980	CB	THR	744	8.228	14.930	-25.334	1.00	122.15	D
	3981	OG1	THR	744	8.139	16.208	-25.970	1.00	122.30	D
45	3982	CG2	THR	744	7.487	13.903	-26.177	1.00	122.06	D
	3983	C	THR	744	8.741	14.707	-22.920	1.00	121.24	D
	3984	O	THR	744	8.856	13.595	-22.399	1.00	120.96	D
50	3985	N	MET	745	9.549	15.732	-22.654	1.00	120.64	D
	3986	CA	MET	745	10.672	15.622	-21.737	1.00	120.07	D
	3987	CB	MET	745	11.523	16.881	-21.791	1.00	120.38	D
	3988	CG	MET	745	12.995	16.582	-21.729	1.00	120.61	D
55	3989	SD	MET	745	13.895	17.821	-22.630	1.00	121.79	D
	3990	CE	MET	745	14.003	17.040	-24.248	1.00	121.33	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3991	C	MET	745	10.191	15.375	-20.318	1.00	119.16	D
	3992	O	MET	745	10.806	14.616	-19.571	1.00	119.47	D
10	3993	N	SER	746	9.109	16.041	-19.942	1.00	117.72	D
	3994	CA	SER	746	8.517	15.831	-18.627	1.00	116.53	D
	3995	CB	SER	746	8.322	14.328	-18.392	1.00	116.85	D
15	3996	OG	SER	746	7.499	13.735	-19.384	1.00	117.32	D
	3997	C	SER	746	9.189	16.409	-17.376	1.00	115.35	D
	3998	O	SER	746	8.905	15.921	-16.282	1.00	115.42	D
	3999	N	ILE	747	10.063	17.403	-17.490	1.00	113.39	D
20	4000	CA	ILE	747	10.676	17.964	-16.278	1.00	111.23	D
	4001	CB	ILE	747	12.094	18.519	-16.557	1.00	111.42	D
	4002	CG2	ILE	747	12.783	18.904	-15.243	1.00	110.85	D
25	4003	CG1	ILE	747	12.935	17.448	-17.254	1.00	111.16	D
	4004	CD1	ILE	747	14.181	17.984	-17.879	1.00	111.76	D
	4005	C	ILE	747	9.747	19.085	-15.788	1.00	109.87	D
	4006	O	ILE	747	9.137	19.766	-16.607	1.00	109.61	D
30	4007	N	GLU	748	9.640	19.276	-14.474	1.00	108.51	D
	4008	CA	GLU	748	8.734	20.295	-13.913	1.00	107.39	D
	4009	CB	GLU	748	7.711	19.600	-12.988	1.00	109.23	D
35	4010	CG	GLU	748	6.248	19.527	-13.495	1.00	111.40	D
	4011	CD	GLU	748	5.994	18.463	-14.571	1.00	112.97	D
	4012	OE1	GLU	748	6.115	17.248	-14.275	1.00	113.35	D
	4013	OE2	GLU	748	5.662	18.848	-15.719	1.00	113.44	D
40	4014	C	GLU	748	9.369	21.484	-13.147	1.00	105.43	D
	4015	O	GLU	748	10.173	21.279	-12.241	1.00	104.77	D
	4016	N	PHE	749	8.982	22.716	-13.505	1.00	103.47	D
45	4017	CA	PHE	749	9.480	23.942	-12.843	1.00	101.74	D
	4018	CB	PHE	749	9.757	25.045	-13.883	1.00	100.69	D
	4019	CG	PHE	749	10.476	24.565	-15.115	1.00	100.55	D
	4020	CD1	PHE	749	11.843	24.716	-15.251	1.00	99.85	D
50	4021	CD2	PHE	749	9.778	23.929	-16.126	1.00	100.99	D
	4022	CE1	PHE	749	12.479	24.254	-16.373	1.00	100.32	D
	4023	CE2	PHE	749	10.434	23.445	-17.259	1.00	101.43	D
55	4024	CZ	PHE	749	11.784	23.600	-17.388	1.00	100.64	D
	4025	C	PHE	749	8.407	24.441	-11.841	1.00	100.85	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
4026	O	PHE	749	7.214	24.417	-12.153	1.00	100.84	D
4027	N	PRO	750	8.810	24.926	-10.648	1.00	99.97	D
4028	CD	PRO	750	10.177	25.299	-10.225	1.00	99.64	D
4029	CA	PRO	750	7.833	25.398	-9.656	1.00	99.71	D
4030	CB	PRO	750	8.692	25.643	-8.426	1.00	98.99	D
4031	CG	PRO	750	9.921	26.205	-9.021	1.00	98.91	D
4032	C	PRO	750	7.045	26.641	-10.059	1.00	99.72	D
4033	O	PRO	750	7.082	27.064	-11.209	1.00	99.97	D
4034	N	GLU	751	6.329	27.216	-9.095	1.00	99.33	D
4035	CA	GLU	751	5.531	28.418	-9.330	1.00	98.80	D
4036	CB	GLU	751	4.831	28.844	-8.036	1.00	99.78	D
4037	CG	GLU	751	3.619	28.013	-7.714	1.00	100.77	D
4038	CD	GLU	751	2.597	28.070	-8.830	1.00	101.15	D
4039	OE1	GLU	751	2.945	27.748	-9.985	1.00	101.44	D
4040	OE2	GLU	751	1.443	28.448	-8.555	1.00	101.81	D
4041	C	GLU	751	6.397	29.560	-9.814	1.00	97.74	D
4042	O	GLU	751	6.224	30.073	-10.927	1.00	96.52	D
4043	N	MET	752	7.323	29.954	-8.949	1.00	96.53	D
4044	CA	MET	752	8.229	31.031	-9.258	1.00	95.56	D
4045	CB	MET	752	9.331	31.122	-8.192	1.00	96.57	D
4046	CG	MET	752	9.238	32.386	-7.314	1.00	98.76	D
4047	SD	MET	752	8.453	33.847	-8.124	1.00	100.33	D
4048	CE	MET	752	9.799	34.664	-8.854	1.00	100.14	D
4049	C	MET	752	8.815	30.868	-10.663	1.00	94.50	D
4050	O	MET	752	8.251	31.409	-11.607	1.00	94.59	D
4051	N	LEU	753	9.899	30.113	-10.825	1.00	93.21	D
4052	CA	LEU	753	10.528	29.942	-12.149	1.00	91.78	D
4053	CB	LEU	753	11.487	28.764	-12.166	1.00	90.35	D
4054	CG	LEU	753	12.819	28.895	-11.456	1.00	89.15	D
4055	CD1	LEU	753	12.644	29.374	-10.035	1.00	88.34	D
4056	CD2	LEU	753	13.457	27.539	-11.491	1.00	88.65	D
4057	C	LEU	753	9.593	29.749	-13.317	1.00	91.44	D
4058	O	LEU	753	9.887	30.188	-14.428	1.00	91.23	D
4059	N	ALA	754	8.487	29.066	-13.082	1.00	91.90	D
4060	CA	ALA	754	7.531	28.820	-14.147	1.00	93.06	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4061	CB	ALA	754	6.399	27.933	-13.633	1.00	92.79	D
	4062	C	ALA	754	6.964	30.111	-14.759	1.00	93.82	D
10	4063	O	ALA	754	6.846	30.200	-15.981	1.00	93.25	D
	4064	N	GLU	755	6.633	31.101	-13.914	1.00	94.99	D
	4065	CA	GLU	755	6.051	32.400	-14.331	1.00	96.19	D
15	4066	CB	GLU	755	5.422	33.117	-13.095	1.00	98.50	D
	4067	CG	GLU	755	4.302	34.197	-13.363	1.00	101.75	D
	4068	CD	GLU	755	2.905	33.824	-12.782	1.00	103.89	D
	4069	OE1	GLU	755	2.461	32.671	-12.992	1.00	104.62	D
20	4070	OE2	GLU	755	2.244	34.678	-12.134	1.00	103.97	D
	4071	C	GLU	755	7.081	33.324	-15.006	1.00	95.52	D
	4072	O	GLU	755	6.794	33.972	-16.019	1.00	95.25	D
25	4073	N	ILE	756	8.281	33.373	-14.431	1.00	94.75	D
	4074	CA	ILE	756	9.363	34.199	-14.948	1.00	93.22	D
	4075	CB	ILE	756	10.523	34.227	-13.969	1.00	92.05	D
	4076	CG2	ILE	756	11.499	35.314	-14.336	1.00	90.95	D
30	4077	CG1	ILE	756	9.994	34.519	-12.577	1.00	91.74	D
	4078	CD1	ILE	756	11.064	34.473	-11.556	1.00	92.95	D
	4079	C	ILE	756	9.834	33.633	-16.273	1.00	93.44	D
35	4080	O	ILE	756	10.051	34.383	-17.224	1.00	93.81	D
	4081	N	ILE	757	10.003	32.315	-16.353	1.00	93.62	D
	4082	CA	ILE	757	10.420	31.750	-17.627	1.00	93.95	D
	4083	CB	ILE	757	10.494	30.209	-17.588	1.00	91.75	D
40	4084	CG2	ILE	757	10.756	29.669	-18.975	1.00	90.90	D
	4085	CG1	ILE	757	11.662	29.777	-16.699	1.00	91.48	D
	4086	CD1	ILE	757	11.660	28.320	-16.315	1.00	91.10	D
45	4087	C	ILE	757	9.367	32.228	-18.623	1.00	95.85	D
	4088	O	ILE	757	9.673	33.038	-19.497	1.00	95.78	D
	4089	N	THR	758	8.127	31.764	-18.448	1.00	98.52	D
	4090	CA	THR	758	6.979	32.135	-19.294	1.00	100.72	D
50	4091	CB	THR	758	5.662	31.878	-18.565	1.00	100.17	D
	4092	OG1	THR	758	5.839	32.147	-17.172	1.00	99.25	D
	4093	CG2	THR	758	5.203	30.454	-18.766	1.00	100.59	D
55	4094	C	THR	758	6.944	33.598	-19.713	1.00	102.85	D
	4095	O	THR	758	6.645	33.923	-20.865	1.00	103.24	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
4096	N	ASN	759	7.210	34.481	-18.761	1.00	104.57	D
4097	CA	ASN	759	7.213	35.896	-19.060	1.00	106.54	D
4098	CB	ASN	759	7.334	36.708	-17.770	1.00	107.18	D
4099	CG	ASN	759	7.717	38.146	-18.032	1.00	108.22	D
4100	OD1	ASN	759	7.420	38.700	-19.092	1.00	108.54	D
4101	ND2	ASN	759	8.376	38.768	-17.058	1.00	108.86	D
4102	C	ASN	759	8.356	36.251	-20.000	1.00	107.90	D
4103	O	ASN	759	8.145	36.866	-21.041	1.00	108.22	D
4104	N	GLN	760	9.566	35.838	-19.641	1.00	109.61	D
4105	CA	GLN	760	10.746	36.144	-20.438	1.00	111.29	D
4106	CB	GLN	760	12.011	35.838	-19.632	1.00	111.83	D
4107	CG	GLN	760	12.186	36.680	-18.385	1.00	113.09	D
4108	CD	GLN	760	12.179	38.167	-18.681	1.00	113.70	D
4109	OE1	GLN	760	12.858	38.636	-19.599	1.00	114.19	D
4110	NE2	GLN	760	11.419	38.924	-17.896	1.00	113.41	D
4111	C	GLN	760	10.891	35.473	-21.799	1.00	112.18	D
4112	O	GLN	760	11.477	36.061	-22.708	1.00	111.69	D
4113	N	ILE	761	10.367	34.259	-21.953	1.00	113.58	D
4114	CA	ILE	761	10.535	33.528	-23.207	1.00	115.12	D
4115	CB	ILE	761	9.503	32.391	-23.353	1.00	114.35	D
4116	CG2	ILE	761	9.809	31.596	-24.622	1.00	114.19	D
4117	CG1	ILE	761	9.552	31.469	-22.123	1.00	113.79	D
4118	CD1	ILE	761	10.328	30.173	-22.312	1.00	113.02	D
4119	C	ILE	761	10.548	34.363	-24.495	1.00	116.87	D
4120	O	ILE	761	11.522	34.313	-25.248	1.00	116.74	D
4121	N	PRO	762	9.484	35.145	-24.769	1.00	118.80	D
4122	CD	PRO	762	8.257	35.427	-24.001	1.00	119.13	D
4123	CA	PRO	762	9.517	35.936	-26.007	1.00	120.40	D
4124	CB	PRO	762	8.115	36.547	-26.059	1.00	119.76	D
4125	CG	PRO	762	7.785	36.732	-24.614	1.00	119.02	D
4126	C	PRO	762	10.620	36.994	-26.021	1.00	122.03	D
4127	O	PRO	762	11.647	36.822	-26.673	1.00	122.16	D
4128	N	LYS	763	10.406	38.073	-25.277	1.00	123.92	D
4129	CA	LYS	763	11.341	39.196	-25.192	1.00	126.19	D
4130	CB	LYS	763	10.961	40.075	-23.995	1.00	125.74	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4131	CG	LYS	763	11.310	39.457	-22.655	1.00	125.82	D
	4132	CD	LYS	763	11.180	40.457	-21.515	1.00	125.86	D
10	4133	CE	LYS	763	9.724	40.759	-21.192	1.00	125.93	D
	4134	NZ	LYS	763	9.571	41.658	-20.007	1.00	125.34	D
	4135	C	LYS	763	12.860	38.919	-25.132	1.00	127.80	D
15	4136	O	LYS	763	13.655	39.762	-25.567	1.00	127.81	D
	4137	N	TYR	764	13.267	37.765	-24.596	1.00	129.73	D
	4138	CA	TYR	764	14.693	37.418	-24.475	1.00	131.28	D
	4139	CB	TYR	764	14.902	36.263	-23.481	1.00	132.18	D
20	4140	CG	TYR	764	15.676	36.665	-22.250	1.00	133.74	D
	4141	CD1	TYR	764	15.034	36.789	-21.018	1.00	134.37	D
	4142	CE1	TYR	764	15.704	37.278	-19.901	1.00	134.88	D
25	4143	CD2	TYR	764	17.024	37.026	-22.333	1.00	134.58	D
	4144	CE2	TYR	764	17.707	37.520	-21.218	1.00	135.24	D
	4145	CZ	TYR	764	17.036	37.647	-20.007	1.00	135.32	D
	4146	OH	TYR	764	17.675	38.185	-18.917	1.00	135.01	D
30	4147	C	TYR	764	15.368	37.017	-25.772	1.00	131.67	D
	4148	O	TYR	764	16.127	37.783	-26.367	1.00	131.64	D
	4149	N	SER	765	15.083	35.780	-26.172	1.00	132.33	D
35	4150	CA	SER	765	15.635	35.159	-27.370	1.00	132.82	D
	4151	CB	SER	765	14.650	34.105	-27.914	1.00	133.31	D
	4152	OG	SER	765	13.399	34.665	-28.285	1.00	133.84	D
	4153	C	SER	765	16.065	36.119	-28.483	1.00	132.44	D
40	4154	O	SER	765	17.177	36.004	-29.004	1.00	132.68	D
	4155	N	ASN	766	15.198	37.067	-28.832	1.00	131.53	D
	4156	CA	ASN	766	15.490	38.038	-29.891	1.00	130.64	D
45	4157	CB	ASN	766	14.310	38.993	-30.082	1.00	131.00	D
	4158	CG	ASN	766	13.031	38.461	-29.492	1.00	131.52	D
	4159	OD1	ASN	766	12.942	38.226	-28.287	1.00	131.69	D
	4160	ND2	ASN	766	12.023	38.272	-30.334	1.00	132.24	D
50	4161	C	ASN	766	16.739	38.884	-29.629	1.00	129.71	D
	4162	O	ASN	766	17.771	38.718	-30.286	1.00	129.98	D
	4163	N	GLY	767	16.615	39.807	-28.673	1.00	128.24	D
55	4164	CA	GLY	767	17.712	40.697	-28.317	1.00	125.71	D
	4165	C	GLY	767	17.254	42.145	-28.215	1.00	123.58	D

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
4166	O	GLY	767	18.001	43.076	-28.523	1.00	123.67	D
4167	N	ASN	768	16.013	42.326	-27.761	1.00	121.21	D
4168	CA	ASN	768	15.382	43.638	-27.618	1.00	117.93	D
4169	CB	ASN	768	13.907	43.490	-28.011	1.00	118.56	D
4170	CG	ASN	768	13.661	42.254	-28.898	1.00	119.51	D
4171	OD1	ASN	768	12.763	41.449	-28.629	1.00	119.65	D
4172	ND2	ASN	768	14.463	42.109	-29.953	1.00	119.47	D
4173	C	ASN	768	15.529	44.166	-26.171	1.00	115.24	D
4174	O	ASN	768	14.715	44.963	-25.687	1.00	115.25	D
4175	N	ILE	769	16.599	43.698	-25.517	1.00	111.53	D
4176	CA	ILE	769	16.996	44.010	-24.130	1.00	106.35	D
4177	CB	ILE	769	17.010	42.700	-23.276	1.00	106.72	D
4178	CG2	ILE	769	18.139	42.736	-22.253	1.00	105.96	D
4179	CG1	ILE	769	15.637	42.466	-22.633	1.00	107.12	D
4180	CD1	ILE	769	15.483	41.092	-21.955	1.00	106.83	D
4181	C	ILE	769	18.427	44.586	-24.175	1.00	102.35	D
4182	O	ILE	769	19.226	44.166	-25.013	1.00	101.64	D
4183	N	LYS	770	18.767	45.512	-23.283	1.00	97.33	D
4184	CA	LYS	770	20.114	46.079	-23.315	1.00	92.92	D
4185	CB	LYS	770	20.057	47.599	-23.311	1.00	92.48	D
4186	CG	LYS	770	21.417	48.285	-23.326	1.00	91.34	D
4187	CD	LYS	770	21.191	49.751	-23.030	1.00	91.61	D
4188	CE	LYS	770	22.458	50.541	-22.808	1.00	91.57	D
4189	NZ	LYS	770	22.092	51.940	-22.420	1.00	90.52	D
4190	C	LYS	770	21.066	45.627	-22.216	1.00	90.16	D
4191	O	LYS	770	21.028	46.128	-21.090	1.00	89.69	D
4192	N	LYS	771	21.932	44.690	-22.579	1.00	86.93	D
4193	CA	LYS	771	22.933	44.147	-21.675	1.00	83.50	D
4194	CB	LYS	771	23.574	42.904	-22.294	1.00	82.69	D
4195	CG	LYS	771	22.605	41.810	-22.745	1.00	82.70	D
4196	CD	LYS	771	23.387	40.601	-23.265	1.00	83.42	D
4197	CE	LYS	771	22.882	40.087	-24.616	1.00	84.30	D
4198	NZ	LYS	771	21.669	39.229	-24.522	1.00	85.18	D
4199	C	LYS	771	24.018	45.201	-21.475	1.00	81.53	D
4200	O	LYS	771	24.694	45.568	-22.429	1.00	82.12	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4201	N	LEU	772	24.186	45.699	-20.255	1.00	78.85	D
	4202	CA	LEU	772	25.231	46.689	-20.003	1.00	76.42	D
10	4203	CB	LEU	772	25.041	47.322	-18.636	1.00	74.60	D
	4204	CG	LEU	772	23.598	47.702	-18.351	1.00	73.45	D
	4205	CD1	LEU	772	23.524	48.369	-17.001	1.00	73.02	D
15	4206	CD2	LEU	772	23.085	48.628	-19.433	1.00	72.99	D
	4207	C	LEU	772	26.570	45.963	-20.024	1.00	75.82	D
	4208	O	LEU	772	26.662	44.825	-19.574	1.00	76.10	D
	4209	N	LEU	773	27.610	46.601	-20.539	1.00	74.99	D
20	4210	CA	LEU	773	28.918	45.951	-20.573	1.00	74.05	D
	4211 1	CB	LEU	773	29.267	45.552	-22.010	1.00	72.45	D
	4212	CG	LEU	773	28.437	44.416	-22.609	1.00	71.06	D
25	4213	CD1	LEU	773	29.066	43.982	-23.912	1.00	71.54	D
	4214	CD2	LEU	773	28.400	43.230	-21.661	1.00	70.94	D
	4215	C	LEU	773	30.004	46.862	-20.008	1.00	74.26	D
	4216	O	LEU	773	29.873	48.077	-20.072	1.00	73.55	D
30	4217	N	PHE	774	31.059	46.285	-19.429	1.00	75.24	D
	4218	CA	PHE	774	32.150	47.111	-18.900	1.00	76.92	D
	4219	CB	PHE	774	32.838	46.449	-17.713	1.00	73.36	D
35	4220	CG	PHE	774	32.052	46.531	-16.459	1.00	69.34	D
	4221	CD1	PHE	774	32.009	47.707	-15.728	1.00	67.48	D
	4222	CD2	PHE	774	31.282	45.461	-16.055	1.00	67.60	D
	4223	CE1	PHE	774	31.204	47.812	-14.611	1.00	66.27	D
40	4224	CE2	PHE	774	30.478	45.558	-14.942	1.00	67.12	D
	4225	CZ	PHE	774	30.433	46.734	-14.219	1.00	66.31	D
	4226	C	PHE	774	33.172	47.334	-19.988	1.00	80.21	D
45	4227	O	PHE	774	33.761	48.404	-20.093	1.00	81.43	D
	4228	N	HIS	775	33.377	46.298	-20.792	1.00	83.76	D
	4229	CA	HIS	775	34.315	46.337	-21.900	1.00	87.34	D
	4230	CB	HIS	775	35.406	45.269	-21.716	1.00	87.97	D
50	4231	CG	HIS	775	36.023	45.254	-20.355	1.00	89.06	D
	4232	CD2	HIS	775	36.094	44.285	-19.412	1.00	89.60	D
	4233	ND1	HIS	775	36.681	46.347	-19.817	1.00	89.65	D
55	4234	CE1	HIS	775	37.127	46.045	-18.614	1.00	90.20	D
	4235	NE2	HIS	775	36.781	44.793	-18.343	1.00	90.43	D

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4236	C	HIS	775	33.501	46.008	-23.154	1.00	90.31	D
	4237	O	HIS	775	32.754	45.028	-23.157	1.00	90.35	D
10	4238	N	GLN	776	33.632	46.820	-24.204	1.00	94.37	D
	4239	CA	GLN	776	32.908	46.573	-25.460	1.00	98.31	D
	4240	CB	GLN	776	32.564	47.907	-26.159	1.00	98.95	D
15	4241	CG	GLN	776	33.657	48.474	-27.093	1.00	101.45	D
	4242	CD	GLN	776	33.554	47.974	-28.542	1.00	102.22	D
	4243	OE1	GLN	776	34.518	48.065	-29.312	1.00	101.71	D
	4244	NE2	GLN	776	32.381	47.461	-28.917	1.00	102.39	D
20	4245	C	GLN	776	33.792	45.706	-26.379	1.00	100.33	D
	4246	O	GLN	776	34.989	45.974	-26.503	1.00	100.20	D
	4247	N	LYS	777	33.216	44.672	-27.002	1.00	102.72	D
25	4248	CA	LYS	777	33.980	43.789	-27.907	1.00	104.94	D
	4249	CB	LYS	777	33.202	42.488	-28.214	1.00	105.65	D
	4250	CG	LYS	777	33.654	41.700	-29.491	1.00	107.33	D
	4251	CD	LYS	777	35.101	41.162	-29.441	1.00	108.50	D
30	4252	CE	LYS	777	35.521	40.502	-30.770	1.00	108.49	D
	4253	NZ	LYS	777	35.344	41.407	-31.944	1.00	109.12	D
	4254	C	LYS	777	34.319	44.498	-29.219	1.00	105.76	D
35	4255	O	LYS	777	35.517	44.512	-29.589	1.00	105.96	D
	4256	OXT	LYS	777	33.383	45.021	-29.864	1.00	106.30	D
	4257	CB	LYS	740	-1.776	39.602	-15.630	1.00	141.89	E
	4258	CG	LYS	740	-2.166	39.561	-14.148	1.00	142.72	E
40	4259	CD	LYS	740	-3.686	39.652	-13.989	1.00	143.70	E
	4260	CE	LYS	740	-4.115	39.873	-12.539	1.00	144.27	E
	4261	NZ	LYS	740	-5.554	40.272	-12.441	1.00	144.10	E
45	4262	C	LYS	740	0.614	38.879	-15.391	1.00	140.04	E
	4263	O	LYS	740	0.331	38.231	-14.381	1.00	139.91	E
	4264	N	LYS	740	-0.112	40.246	-17.356	1.00	141.08	E
	4265	CA	LYS	740	-0.313	39.979	-15.902	1.00	140.87	E
50	4266	N	GLU	741	1.719	38.664	-16.097	1.00	138.85	E
	4267	CA	GLU	741	2.688	37.662	-15.678	1.00	137.18	E
	4268	CB	GLU	741	3.798	37.516	-16.727	1.00	138.20	E
55	4269	CG	GLU	741	4.326	36.108	-16.872	1.00	139.42	E
	4270	CD	GLU	741	3.287	35.187	-17.456	1.00	140.29	E

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4271	OE1	GLU	741	2.190	35.093	-16.867	1.00	140.93	E
	4272	OE2	GLU	741	3.559	34.562	-18.502	1.00	140.86	E
10	4273	C	GLU	741	3.290	38.208	-14.386	1.00	134.99	E
	4274	O	GLU	741	3.029	39.350	-14.006	1.00	134.69	E
	4275	N	ASN	742	4.084	37.385	-13.708	1.00	132.25	E
15	4276	CA	ASN	742	4.755	37.799	-12.483	1.00	129.12	E
	4277	CB	ASN	742	5.828	38.841	-12.837	1.00	130.35	E
	4278	CG	ASN	742	6.642	38.448	-14.068	1.00	130.69	E
	4279	OD1	ASN	742	6.467	39.011	-15.150	1.00	130.62	E
20	4280	ND2	ASN	742	7.525	37.466	-13.906	1.00	130.78	E
	4281	C	ASN	742	3.846	38.329	-11.365	1.00	126.11	E
	4282	O	ASN	742	4.167	39.325	-10.706	1.00	125.74	E
25	4283	N	ALA	743	2.718	37.661	-11.156	1.00	122.24	E
	4284	CA	ALA	743	1.797	38.047	-10.095	1.00	117.75	E
	4285	CB	ALA	743	0.469	37.301	-10.236	1.00	118.53	E
	4286	C	ALA	743	2.469	37.695	-8.769	1.00	114.59	E
30	4287	O	ALA	743	2.385	38.455	-7.806	1.00	114.16	E
	4288	N	LEU	744	3.154	36.553	-8.717	1.00	110.51	E
	4289	CA	LEU	744	3.823	36.170	-7.480	1.00	106.08	E
35	4290	CB	LEU	744	4.327	34.718	-7.543	1.00	105.35	E
	4291	CG	LEU	744	4.090	33.917	-6.245	1.00	104.62	E
	4292	CD1	LEU	744	4.547	32.469	-6.396	1.00	103.98	E
	4293	CD2	LEU	744	4.827	34.584	-5.099	1.00	104.60	E
40	4294	C	LEU	744	4.973	37.134	-7.143	1.00	103.50	E
	4295	O	LEU	744	5.201	37.421	-5.971	1.00	103.23	E
	4296	N	LEU	745	5.682	37.650	-8.151	1.00	100.22	E
45	4297	CA	LEU	745	6.791	38.587	-7.894	1.00	97.11	E
	4298	CB	LEU	745	7.598	38.878	-9.172	1.00	95.13	E
	4299	CG	LEU	745	9.114	38.639	-9.295	1.00	92.39	E
	4300	CD1	LEU	745	9.534	39.232	-10.627	1.00	91.20	E
50	4301	CD2	LEU	745	9.924	39.266	-8.162	1.00	90.98	E
	4302	C	LEU	745	6.295	39.921	-7.340	1.00	95.69	E
	4303	O	LEU	745	6.781	40.383	-6.305	1.00	95.37	E
55	4304	N	ARG	746	5.340	40.553	-8.026	1.00	94.08	E
	4305	CA	ARG	746	4.847	41.827	-7.528	1.00	91.98	E

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
4306	CB	ARG	746	3.666	42.370	-8.359	1.00	92.78	E
4307	CG	ARG	746	3.300	43.811	-7.933	1.00	95.34	E
4308	CD	ARG	746	2.281	44.580	-8.816	1.00	96.94	E
4309	NE	ARG	746	2.756	45.145	-10.091	1.00	99.07	E
4310	CZ	ARG	746	2.598	44.566	-11.287	1.00	100.49	E
4311	NH1	ARG	746	1.992	43.386	-11.381	1.00	100.23	E
4312	NH2	ARG	746	2.962	45.204	-12.397	1.00	100.52	E
4313	C	ARG	746	4.439	41.650	-6.072	1.00	90.46	E
4314	O	ARG	746	4.742	42.493	-5.237	1.00	89.72	E
4315	N	TYR	747	3.785	40.536	-5.754	1.00	89.44	E
4316	CA	TYR	747	3.362	40.281	-4.379	1.00	88.36	E
4317	CB	TYR	747	2.558	38.960	-4.304	1.00	86.74	E
4318	CG	TYR	747	2.370	38.390	-2.904	1.00	85.09	E
4319	CD1	TYR	747	1.515	38.992	-1.981	1.00	84.23	E
4320	CE1	TYR	747	1.416	38.512	-0.669	1.00	84.20	E
4321	CD2	TYR	747	3.110	37.283	-2.487	1.00	84.97	E
4322	CE2	TYR	747	3.020	36.801	-1.187	1.00	84.52	E
4323	CZ	TYR	747	2.179	37.422	-0.280	1.00	84.47	E
4324	OH	TYR	747	2.144	36.982	1.024	1.00	84.78	E
4325	C	TYR	747	4.571	40.244	-3.431	1.00	88.64	E
4326	O	TYR	747	4.569	40.907	-2.394	1.00	88.55	E
4327	N	LEU	748	5.602	39.494	-3.810	1.00	89.68	E
4328	CA	LEU	748	6.813	39.348	-2.999	1.00	89.96	E
4329	CB	LEU	748	7.723	38.291	-3.635	1.00	88.64	E
4330	CG	LEU	748	7.137	36.874	-3.615	1.00	87.96	E
4331	CD1	LEU	748	7.795	36.025	-4.684	1.00	87.83	E
4332	CD2	LEU	748	7.322	36.254	-2.236	1.00	86.92	E
4333	C	LEU	748	7.592	40.642	-2.778	1.00	90.99	E
4334	O	LEU	748	8.220	40.826	-1.734	1.00	90.21	E
4335	N	LEU	749	7.535	41.541	-3.758	1.00	93.07	E
4336	CA	LEU	749	8.243	42.816	-3.678	1.00	95.67	E
4337	CB	LEU	749	8.470	43.365	-5.094	1.00	92.83	E
4338	CG	LEU	749	9.614	42.671	-5.837	1.00	90.56	E
4339	CD1	LEU	749	9.654	43.080	-7.295	1.00	88.14	E
4340	CD2	LEU	749	10.916	43.016	-5.133	1.00	89.43	E

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4341	C	LEU	749	7.578	43.886	-2.811	1.00	98.99	E
	4342	O	LEU	749	8.202	44.904	-2.501	1.00	99.50	E
10	4343	N	ASP	750	6.330	43.648	-2.404	1.00	103.16	E
	4344	CA	ASP	750	5.579	44.607	-1.587	1.00	107.11	E
	4345	CB	ASP	750	4.152	44.727	-2.135	1.00	106.92	E
15	4346	CG	ASP	750	4.053	45.700	-3.301	1.00	107.42	E
	4347	OD1	ASP	750	4.995	45.742	-4.122	1.00	107.42	E
	4348	OD2	ASP	750	3.034	46.421	-3.408	1.00	107.60	E
	4349	C	ASP	750	5.542	44.392	-0.063	1.00	110.57	E
20	4350	O	ASP	750	5.804	45.327	0.692	1.00	110.50	E
	4351	N	LYS	751	5.227	43.182	0.398	1.00	114.91	E
	4352	CA	LYS	751	5.157	42.897	1.845	1.00	119.84	E
25	4353	CB	LYS	751	4.738	41.430	2.053	1.00	120.51	E
	4354	CG	LYS	751	5.442	40.409	1.165	1.00	121.28	E
	4355	CD	LYS	751	5.130	39.006	1.655	1.00	122.93	E
	4356	CE	LYS	751	5.522	38.865	3.125	1.00	124.03	E
30	4357	NZ	LYS	751	4.915	37.676	3.787	1.00	124.84	E
	4358	C	LYS	751	6.425	43.218	2.677	1.00	122.73	E
	4359	O	LYS	751	7.049	44.262	2.478	1.00	122.86	E
35	4360	N	ASP	752	6.765	42.351	3.641	1.00	126.13	E
	4361	CA	ASP	752	7.964	42.504	4.492	1.00	129.40	E
	4362	CB	ASP	752	9.183	42.759	3.586	1.00	130.18	E
	4363	CG	ASP	752	10.443	42.073	4.084	1.00	131.66	E
40	4364	OD1	ASP	752	10.786	42.244	5.275	1.00	132.08	E
	4365	OD2	ASP	752	11.097	41.367	3.281	1.00	132.63	E
	4366	C	ASP	752	7.960	43.562	5.638	1.00	130.58	E
45	4367	O	ASP	752	7.487	44.684	5.459	1.00	131.17	E
	4368	N	ASP	753	8.496	43.162	6.807	1.00	132.38	E
	4369	CA	ASP	753	8.673	43.970	8.046	1.00	133.53	E
	4370	CB	ASP	753	7.392	44.726	8.497	1.00	134.59	E
50	4371	CG	ASP	753	7.602	45.573	9.796	1.00	134.88	E
	4372	OD1	ASP	753	7.631	45.005	10.915	1.00	135.11	E
	4373	OD2	ASP	753	7.740	46.814	9.695	1.00	134.97	E
55	4374	C	ASP	753	9.092	43.000	9.154	1.00	133.95	E
	4375	O	ASP	753	10.293	42.981	9.496	1.00	134.41	E

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
4376	OXT	ASP	753	8.223	42.246	9.644	1.00	134.72	E
4377	C1	FLU	1	31.469	6.647	9.774	1.00	68.41	C
4378	C2	FLU	1	31.819	7.274	8.637	1.00	66.97	C
4379	C3	FLU	1	33.096	8.036	8.648	1.00	68.13	C
4380	C4	FLU	1	33.846	8.156	9.949	1.00	67.54	C
4381	C5	FLU	1	33.446	7.519	11.039	1.00	68.42	C
4382	C6	FLU	1	34.232	7.698	12.303	1.00	69.88	C
4383	F61	FLU	1	35.211	8.643	12.190	1.00	71.79	C
4384	C7	FLU	1	33.332	8.128	13.460	1.00	70.88	C
4385	C8	FLU	1	32.025	7.330	13.516	1.00	72.02	C
4386	C9	FLU	1	31.297	7.119	12.193	1.00	71.23	C
4387	C10	FLU	1	32.213	6.638	11.065	1.00	69.64	C
4388	C11	FLU	1	29.932	6.437	12.283	1.00	71.39	C
4389	C12	FLU	1	29.105	6.683	13.539	1.00	72.71	C
4390	C13	FLU	1	29.890	6.661	14.857	1.00	73.76	C
4391	C14	FLU	1	31.136	7.539	14.738	1.00	72.68	C
4392	C15	FLU	1	31.614	7.926	16.141	1.00	74.16	C
4393	C16	FLU	1	30.383	7.643	16.996	1.00	74.79	C
4394	C17	FLU	1	29.218	7.330	16.053	1.00	76.56	C
4395	C18	FLU	1	30.305	5.197	15.044	1.00	73.36	C
4396	C19	FLU	1	32.695	5.192	11.181	1.00	69.59	C
4397	C20	FLU	1	28.267	6.341	16.712	1.00	77.91	C
4398	S21	FLU	1	26.498	6.507	16.475	1.00	78.08	C
4399	C21	FLU	1	25.978	4.792	16.637	1.00	79.64	C
4400	F21	FLU	1	26.415	4.104	15.543	1.00	82.24	C
4401	C22	FLU	1	30.250	8.586	18.187	1.00	74.40	C
4402	P1	FLU	1	30.899	8.375	11.854	1.00	74.42	C
4403	O1	FLU	1	33.524	8.563	7.621	1.00	70.89	C
4404	O2	FLU	1	30.058	5.029	12.153	1.00	70.24	C
4405	O3	FLU	1	28.413	8.454	15.697	1.00	79.76	C
4406	O4	FLU	1	28.685	5.416	17.406	1.00	79.85	C
4407	C	FLU	1	28.738	9.781	15.735	1.00	81.43	C
4408	CC	FLU	1	27.622	10.758	15.411	1.00	80.02	C
4409	CC3	FLU	1	27.540	10.867	13.889	1.00	78.83	C
4410	O	FLU	1	29.829	10.282	16.003	1.00	82.80	C

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4411	C1	FLU	2	18.731	25.721	-9.807	1.00	66.81	F
	4412	C2	FLU	2	19.386	25.696	-8.652	1.00	65.83	F
10	4413	C3	FLU	2	20.603	26.567	-8.540	1.00	66.00	F
	4414	C4	FLU	2	21.052	27.321	-9.758	1.00	65.97	F
	4415	C5	FLU	2	20.346	27.301	-10.888	1.00	66.75	F
15	4416	C6	FLU	2	20.870	28.079	-12.060	1.00	67.70	F
	4417	F61	FLU	2	22.113	28.603	-11.869	1.00	67.61	F
	4418	C7	FLU	2	20.975	27.192	-13.299	1.00	67.74	F
	4419	C8	FLU	2	19.740	26.304	-13.471	1.00	70.03	F
20	4420	C9	FLU	2	19.217	25.580	-12.225	1.00	69.01	F
	4421	C10	FLU	2	19.073	26.521	-11.026	1.00	67.85	F
	4422	C11	FLU	2	18.071	24.593	-12.461	1.00	69.61	F
25	4423	C12	FLU	2	18.023	23.880	-13.813	1.00	72.06	F
	4424	C13	FLU	2	18.345	24.746	-15.029	1.00	73.82	F
	4425	C14	FLU	2	19.647	25.492	-14.762	1.00	72.07	F
	4426	C15	FLU	2	20.287	25.940	-16.075	1.00	73.54	F
30	4427	C16	FLU	2	19.659	24.961	-17.062	1.00	74.63	F
	4428	C17	FLU	2	18.758	23.991	-16.287	1.00	77.21	F
	4429	C18	FLU	2	17.155	25.681	-15.219	1.00	72.30	F
35	4430	C19	FLU	2	17.921	27.513	-11.113	1.00	68.89	F
	4431	C20	FLU	2	17.540	23.530	-17.071	1.00	79.04	F
	4432	S21	FLU	2	16.760	21.975	-16.623	1.00	81.55	F
	4433	C21	FLU	2	15.234	22.064	-17.575	1.00	83.80	F
40	4434	F21	FLU	2	14.313	22.715	-16.813	1.00	86.86	F
	4435	C22	FLU	2	20.799	24.580	-17.998	1.00	74.95	F
	4436	F1	FLU	2	20.223	24.708	-11.913	1.00	70.32	F
45	4437	O1	FLU	2	21.233	26.659	-7.481	1.00	68.73	F
	4438	O2	FLU	2	16.816	25.254	-12.348	1.00	69.31	F
	4439	O3	FLU	2	19.455	22.843	-15.815	1.00	80.25	F
	4440	O4	FLU	2	17.083	24.202	-17.994	1.00	79.76	F
50	4441	C	FLU	2	19.977	21.889	-16.658	1.00	82.09	F
	4442	CC	FLU	2	20.497	20.676	-15.905	1.00	81.78	F
	4443	CC3	FLU	2	21.989	20.751	-15.572	1.00	78.23	F
55	4444	O	FLU	2	20.024	21.982	-17.881	1.00	84.06	F
	4445	O	HOH		19.523	33.396	-3.571	1.00	76.62	W

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
			2	42.941	37.375	-17.594	1.00	73.82	W
	O	HOH	3	-5.577	41.115	-21.499	1.00	86.78	W
	O	HOH	4	38.453	47.403	-23.099	1.00	91.58	W
	O	HOH	5	26.829	53.228	-14.715	1.00	76.19	W
	O	HOH	6	27.841	43.647	-16.662	1.00	83.67	W
	O	HOH	7	37.308	4.182	2.628	1.00	82.13	W
	O	HOH	8	51.563	23.152	18.316	1.00	77.47	W
	O	HOH	9	14.159	62.331	-10.476	1.00	72.93	W
	O	HOH	10	41.691	4.638	29.350	1.00	81.82	W
	O	HOH	11	51.782	5.887	14.391	1.00	69.86	W
	O	HOH	12	28.889	-4.501	5.566	1.00	74.77	W
	O	HOH	13	49.515	19.573	17.146	1.00	84.85	W
	O	HOH	14	3.901	51.708	-24.615	1.00	75.63	W
	O	HOH	15	44.526	-5.219	33.428	1.00	92.56	W
	O	HOH	16	49.031	2.748	26.331	1.00	85.58	W
	O	HOH	17	69.550	9.656	-15.186	1.00	95.60	W
	O	HOH	18	37.583	46.290	-30.177	1.00	94.72	W
	O	HOH	19	44.712	-10.424	23.759	1.00	93.68	W
	O	HOH	20	10.095	47.678	8.481	1.00	94.91	W
	O	HOH	21	23.412	55.862	-18.634	1.00	64.40	W
	O	HOH	22	45.467	40.765	-18.463	1.00	82.28	W
	O	HOH	23	63.473	2.606	6.965	1.00	78.36	W
	O	HOH	24	60.128	12.787	22.992	1.00	78.64	W
	O	HOH	25	43.814	-4.792	-2.342	1.00	73.85	W
	O	HOH	26	35.802	58.962	-5.624	1.00	86.33	W
	O	HOH	27	18.584	43.655	-32.292	1.00	110.47	W
	O	HOH	28	1.260	31.718	-15.461	1.00	94.95	W
	O	HOH	29	39.707	25.903	12.225	1.00	81.11	W
	O	HOH	30	8.864	39.637	-26.908	1.00	102.41	W
	O	HOH	31	25.220	8.573	-6.280	1.00	84.78	W
	O	HOH	32	44.012	3.517	19.660	1.00	79.65	W
	O	HOH	33	61.617	5.971	3.196	1.00	76.45	W
	O	HOH	34	33.361	11.235	25.669	1.00	87.33	W
	O	HOH	35	48.747	6.563	26.113	1.00	94.00	W
	O	HOH	36	35.557	39.674	3.256	1.00	84.29	W

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TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4481	O	HOH	37	43.568	3.880	17.239	1.00	80.95	W
	4482	O	HOH	38	-2.757	39.376	-25.950	1.00	94.87	W
10	4483	O	HOH	39	37.467	5.537	29.129	1.00	102.58	W
	4484	O	HOH	40	18.443	9.340	-17.496	1.00	75.91	W
	4485	O	HOH	41	58.946	27.891	16.135	1.00	117.13	W
15	4486	O	HOH	42	29.763	47.759	-26.838	1.00	87.96	W
	4487	O	HOH	43	38.372	-23.387	18.058	1.00	88.20	W
	4488	O	HOH	44	2.160	53.587	-26.952	1.00	103.43	W
	4489	O	HOH	45	15.637	33.354	6.623	1.00	78.76	W
20	4490	O	HOH	46	36.791	8.067	1.836	1.00	92.22	W
	4491	O	HOH	47	41.420	-19.727	12.465	1.00	90.65	W
	4492	O	HOH	48	35.606	42.694	-34.099	1.00	92.07	W
25	4493	O	HOH	49	9.972	40.686	-28.976	1.00	90.64	W
	4494	O	HOH	50	56.197	25.170	9.346	1.00	102.45	W
	4495	O	HOH	51	45.027	-14.654	-8.801	1.00	73.69	W
	4496	O	HOH	52	1.523	47.124	-14.313	1.00	79.60	W
30	4497	O	HOH	53	48.094	20.357	-1.285	1.00	63.38	W
	4498	O	HOH	54	-3.646	36.748	-23.378	1.00	89.36	W
	4499	O	HOH	55	54.686	-16.296	13.451	1.00	93.02	W
35	4500	O	HOH	56	18.176	19.988	-29.385	1.00	85.25	W
	4501	O	HOH	57	18.017	7.401	19.131	1.00	89.90	W
	4502	O	HOH	58	46.405	10.360	-8.409	1.00	79.17	W
	4503	O	HOH	59	60.377	-2.468	19.274	1.00	93.48	W
40	4504	O	HOH	60	-2.437	45.083	-20.632	1.00	102.27	W
	4505	O	HOH	61	38.901	33.047	-19.920	1.00	80.62	W
	4506	O	HOH	62	28.293	32.129	-28.814	1.00	87.71	W
45	4507	O	HOH	63	44.732	10.741	-4.492	1.00	81.65	W
	4508	O	HOH	64	24.682	4.218	-1.857	1.00	76.04	W
	4509	O	HOH	65	31.637	0.342	25.661	1.00	82.29	W
	4510	O	HOH	66	4.471	24.618	-9.189	1.00	90.31	W
50	4511 1	O	HOH	67	30.941	3.201	26.651	1.00	103.40	W
	4512	O	HOH	68	39.603	1.672	28.491	1.00	113.23	W
	4513	O	HOH	69	30.027	53.782	2.347	1.00	86.93	W
55	4514	O	HOH	70	24.112	8.345	20.698	1.00	83.64	W
	4515	O	HOH	71	11.238	11.421	-10.129	1.00	104.98	W

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
4516	O	HOH	72	10.919	8.389	-11.074	1.00	108.91	W
4517	O	HOH	73	37.382	35.007	1.398	1.00	60.56	W
4518	O	HOH	74	44.332	42.288	-22.956	1.00	99.96	W
4519	O	HOH	75	9.555	39.664	1.611	1.00	103.96	W
4520	O	HOH	76	22.671	31.229	-1.881	1.00	85.23	W
4521	O	HOH	77	4.772	47.026	10.208	1.00	105.31	W
4522	O	HOH	78	50.024	16.208	-4.476	1.00	84.94	W
4523	O	HOH	79	48.969	-19.537	13.191	1.00	101.64	W
4524	O	HOH	80	9.808	51.313	-0.626	1.00	83.97	W
4525	O	HOH	81	57.763	14.751	31.604	1.00	84.36	W
4526	O	HOH	82	58.922	-4.343	19.998	1.00	97.27	W
4527	O	HOH	83	53.567	-16.970	16.934	1.00	74.06	W
4528	O	HOH	84	62.029	10.217	-3.169	1.00	82.95	W
4529	O	HOH	85	50.109	40.904	-11.762	1.00	102.45	W
4530	O	HOH	86	1.821	49.898	-13.245	1.00	99.91	W
4531	O	HOH	87	21.200	13.279	0.465	1.00	79.27	W
4532	O	HOH	88	63.358	-1.153	3.412	1.00	102.97	W
4533	O	HOH	89	18.070	25.741	14.704	1.00	86.42	W
4534	O	HOH	90	60.672	12.708	31.162	1.00	112.67	W
4535	O	HOH	91	13.164	-6.141	17.266	1.00	110.15	W
4536	O	HOH	92	10.846	49.963	-21.798	1.00	90.71	W
4537	O	HOH	93	34.418	24.160	-18.821	1.00	87.02	W
4538	O	HOH	94	18.611 1	25.870	-27.603	1.00	112.94	W
4539	O	HOH	95	5.242	48.331	1.314	1.00	78.27	W
4540	O	HOH	96	43.848	-9.310	18.979	1.00	109.50	W
4541	O	HOH	97	22.575	6.419	-8.204	1.00	80.78	W
4542	O	HOH	98	44.607	25.465	2.534	1.00	86.75	W
4543	O	HOH	99	25.294	0.805	26.895	1.00	79.15	W
4544	O	HOH	100	15.873	13.445	16.080	1.00	65.33	W
4545	O	HOH	101	46.669	-4.925	-3.439	1.00	63.97	W
4546	O	HOH	102	10.476	57.087	-17.694	1.00	73.69	W
4547	O	HOH	103	32.866	39.274	-27.212	1.00	95.95	W
4548	O	HOH	104	42.351	-21.786	13.383	1.00	84.99	W
4549	O	HOH	105	-0.138	38.199	-23.756	1.00	105.98	W
4550	O	HOH	106	28.478	19.343	-28.838	1.00	93.72	W

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT										
5	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
	4551	O	HOH	107	26.576	57.319	-16.982	1.00	115.17	W
	4552	O	HOH	108	65.453	11.244	1.860	1.00	100.82	W
10	4553	O	HOH	109	-0.708	38.981	-21.728	1.00	89.17	W
	4554	O	HOH	110	27.824	-8.474	20.771	1.00	86.00	W
	4555	O	HOH	111 1	39.931	48.171	-29.933	1.00	125.52	W
15	4556	O	HOH	112	45.275	-19.198	12.656	1.00	101.55	W
	4557	O	HOH	113	45.279	29.204	13.170	1.00	81.25	W
	4558	O	HOH	114	39.604	-9.905	-10.328	1.00	73.44	W
	4559	O	HOH	115	64.611	12.168	-0.278	1.00	95.59	W
20	4560	O	HOH	116	68.609	24.621	6.796	1.00	99.37	W
	4561	O	HOH	117	25.054	-7.146	20.234	1.00	85.14	W
	4562	O	HOH	118	46.697	4.148	27.896	1.00	105.02	W
25	4563	O	HOH	119	22.193	26.077	-24.741	1.00	69.48	W
	4564	O	HOH	120	26.353	57.873	-19.525	1.00	108.32	W
	4565	O	HOH	121	8.026	55.457	-17.860	1.00	98.34	W
	4566	O	HOH	122	12.559	11.828	-24.035	1.00	93.10	W
30	4567	O	HOH	123	-4.915	40.336	-23.651	1.00	96.08	W
	4568	O	HOH	124	7.424	56.806	-15.154	1.00	95.41	W
	4569	O	HOH	125	9.243	9.680	-21.618	1.00	88.75	W
35	4570	O	HOH	126	41.604	39.684	-21.569	1.00	113.19	W
	4571	O	HOH	127	39.225	-16.888	3.197	1.00	66.34	W
	4572	O	HOH	128	40.747	40.837	-23.085	1.00	85.74	W
	4573	O	HOH	129	36.354	54.080	16.892	1.00	107.37	W
40	4574	O	HOH	130	40.021	-4.808	33.204	1.00	91.23	W
	4575	O	HOH	131	55.071	24.231	-2.554	1.00	70.80	W
	4576	O	HOH	132	46.616	48.721	-2.372	1.00	83.01	W
45	4577	O	HOH	133	26.663	54.965	-17.649	1.00	94.09	W
	4578	O	HOH	134	60.447	24.164	-2.252	1.00	108.34	W
	4579	O	HOH	135	37.786	54.011	-0.139	1.00	112.49	W
	4580	O	HOH	136	39.669	27.027	16.006	1.00	113.82	W
50	4581	O	HOH	137	54.615	6.585	26.415	1.00	97.63	W
	4582	O	HOH	138	38.455	26.713	14.349	1.00	110.00	W
	4583	O	HOH	139	25.536	31.838	-27.978	1.00	118.35	W
55	4584	O	HOH	140	43.859	28.725	11.124	1.00	88.60	W
	4585	O	HOH	141	39.097	47.972	-32.369	1.00	104.31	W

TABLE 2 (continued)

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF GR α IN COMPLEX WITH FLUTICASONE PROPIONATE AND A TIF2 FRAGMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
4586	O	HOH	142	25.807	33.585	-30.771	1.00	99.66	W
4587	O	HOH	143	39.247	53.006	-1.353	1.00	94.50	W
4588	O	HOH	144	45.655	-13.890	-5.094	1.00	92.07	W
4589	O	HOH	145	34.471	-14.556	13.467	1.00	82.57	W

TABLE 3

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
1	CB	GLN	527	60.207	9.806	35.497	1.00	60.77	
2	CG	GLN	527	60.501	11.318	35.564	1.00	60.74	
3	CD	GLN	527	60.595	11.993	34.172	1.00	63.52	
4	OE1	GLN	527	60.493	13.224	34.058	1.00	61.80	
5	NE2	GLN	527	60.794	11.187	33.121	1.00	61.21	
6	C	GLN	527	62.073	8.590	36.647	1.00	62.83	
7	O	GLN	527	63.240	8.191	36.724	1.00	59.67	
8	N	GLN	527	61.009	7.618	34.618	1.00	58.91	
9	CA	GLN	527	61.426	8.890	35.289	1.00	62.13	
10	N	LEU	528	61.308	8.776	37.716	1.00	62.73	
11	CA	LEU	528	61.816	8.538	39.064	1.00	65.02	
12	CB	LEU	528	62.105	9.889	39.733	1.00	62.65	
13	CG	LEU	528	62.864	10.872	38.813	1.00	59.23	
14	CD1	LEU	528	62.071	12.198	38.675	1.00	63.52	
15	CD2	LEU	528	64.283	11.105	39.356	1.00	60.04	
16	C	LEU	528	60.823	7.690	39.888	1.00	59.38	
17	O	LEU	528	60.586	6.527	39.527	1.00	63.35	
18	N	THR	529	60.247	8.256	40.960	1.00	60.40	
19	CA	THR	529	59.282	7.539	41.835	1.00	60.79	
20	CB	THR	529	57.841	8.227	41.847	1.00	63.67	
21	OG1	THR	529	57.918	9.561	42.382	1.00	60.60	
22	CG2	THR	529	56.867	7.410	42.706	1.00	62.04	
23	C	THR	529	59.134	6.056	41.397	1.00	61.38	
24	O	THR	529	58.454	5.754	40.398	1.00	59.93	
25	N	PRO	530	59.743	5.117	42.163	1.00	61.16	
26	CD	PRO	530	60.110	5.411	43.563	1.00	60.38	
27	CA	PRO	530	59.753	3.660	41.928	1.00	62.39	

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
28	CB	PRO	530	60.388	3.109	43.213	1.00	58.06
29	CG	PRO	530	59.914	4.071	44.249	1.00	64.31
30	C	PRO	530	58.453	2.927	41.537	1.00	63.39
31	O	PRO	530	57.400	3.542	41.363	1.00	59.17
32	N	THR	531	58.554	1.603	41.419	1.00	62.27
33	CA	THR	531	57.455	0.742	40.997	1.00	61.68
34	CB	THR	531	57.989	-0.404	40.058	1.00	60.38
35	OG1	THR	531	57.209	-0.461	38.853	1.00	60.25
36	CG2	THR	531	57.937	-1.760	40.757	1.00	60.67
37	C	THR	531	56.629	0.125	42.117	1.00	60.82
38	O	THR	531	55.533	-0.361	41.864	1.00	62.20
39	N	LEU	532	57.122	0.128	43.348	1.00	60.85
40	CA	LEU	532	56.324	-0.465	44.418	1.00	60.11
41	CB	LEU	532	57.183	-0.775	45.637	1.00	64.22
42	CG	LEU	532	56.388	-1.514	46.704	1.00	63.74
43	CD1	LEU	532	55.677	-2.694	46.082	1.00	62.66
44	CD2	LEU	532	57.317	-1.968	47.806	1.00	63.22
45	C	LEU	532	55.143	0.422	44.817	1.00	62.08
46	O	LEU	532	54.047	-0.075	45.061	1.00	61.27
47	N	VAL	533	55.366	1.733	44.883	1.00	59.27
48	CA	VAL	533	54.297	2.677	45.222	1.00	62.90
49	CB	VAL	533	54.858	4.050	45.638	1.00	64.91
50	CG1	VAL	533	55.572	4.693	44.465	1.00	60.86
51	CG2	VAL	533	53.746	4.941	46.102	1.00	61.00
52	C	VAL	533	53.422	2.874	43.979	1.00	62.21
53	O	VAL	533	52.281	3.321	44.065	1.00	61.72
54	N	SER	534	53.981	2.553	42.817	1.00	60.92
55	CA	SER	534	53.249	2.665	41.564	1.00	61.24
56	CB	SER	534	54.196	2.474	40.386	1.00	61.92
57	OG	SER	534	53.468	2.355	39.183	1.00	61.38
58	C	SER	534	52.209	1.557	41.566	1.00	64.31
59	O	SER	534	51.105	1.691	41.027	1.00	62.62
60	N	LEU	535	52.581	0.452	42.193	1.00	61.91
61	CA	LEU	535	51.697	-0.684	42.288	1.00	60.97
62	CB	LEU	535	52.479	-1.922	42.730	1.00	66.65
63	CG	LEU	535	51.949	-3.225	42.131	1.00	63.58
64	CD1	LEU	535	52.657	-3.505	40.827	1.00	62.14

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
65	CD2	LEU	535	52.175	-4.364	43.090	1.00	61.95
66	C	LEU	535	50.588	-0.353	43.285	1.00	59.91
67	O	LEU	535	49.432	-0.684	43.060	1.00	63.02
68	N	LEU	536	50.933	0.315	44.381	1.00	62.58
69	CA	LEU	536	49.932	0.683	45.376	1.00	59.17
70	CB	LEU	536	50.583	1.413	46.541	1.00	61.74
71	CG	LEU	536	51.501	0.625	47.460	1.00	58.87
72	CD1	LEU	536	51.953	1.545	48.553	1.00	59.54
73	CD2	LEU	536	50.781	-0.575	48.045	1.00	63.64
74	C	LEU	536	48.821	1.569	44.812	1.00	63.31
75	O	LEU	536	47.672	1.489	45.256	1.00	61.67
76	N	GLU	537	49.171	2.415	43.845	1.00	59.21
77	CA	GLU	537	48.231	3.343	43.213	1.00	59.76
78	CB	GLU	537	48.984	4.292	42.302	1.00	59.81
79	CG	GLU	537	48.816	5.744	42.625	1.00	60.10
80	CD	GLU	537	48.907	6.616	41.385	1.00	64.34
81	OE1	GLU	537	47.868	6.813	40.707	1.00	57.41
82	OE2	GLU	537	50.024	7.091	41.084	1.00	62.84
83	C	GLU	537	47.139	2.698	42.371	1.00	61.66
84	O	GLU	537	45.973	3.101	42.433	1.00	60.28
85	N	VAL	538	47.536	1.717	41.564	1.00	60.48
86	CA	VAL	538	46.606	1.045	40.674	1.00	63.41
87	CB	VAL	538	47.325	0.448	39.442	1.00	64.15
88	CG1	VAL	538	48.334	1.444	38.903	1.00	60.29
89	CG2	VAL	538	47.973	-0.883	39.797	1.00	63.88
90	C	VAL	538	45.768	-0.046	41.311	1.00	57.99
91	O	VAL	538	44.828	-0.530	40.683	1.00	58.71
92	N	ILE	539	46.094	-0.454	42.535	1.00	61.14
93	CA	ILE	539	45.282	-1.484	43.186	1.00	60.23
94	CB	ILE	539	46.141	-2.499	44.010	1.00	65.32
95	CG2	ILE	539	47.243	-3.066	43.140	1.00	61.32
96	CG1	ILE	539	46.775	-1.833	45.228	1.00	63.80
97	CD1	ILE	539	47.356	-2.833	46.207	1.00	60.85
98	C	ILE	539	44.259	-0.811	44.097	1.00	61.40
99	O	ILE	539	43.321	-1.447	44.573	1.00	63.49
100	N	GLU	540	44.451	0.489	44.310	1.00	61.12
101	CA	GLU	540	43.584	1.307	45.153	1.00	60.76

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	102	CB	GLU	540	44.109	2.753	45.173	1.00	58.26
	103	CG	GLU	540	43.466	3.684	46.191	1.00	61.15
	104	CD	GLU	540	43.598	3.183	47.619	1.00	61.95
10	105	OE1	GLU	540	44.656	2.591	47.950	1.00	59.71
	106	OE2	GLU	540	42.649	3.397	48.410	1.00	62.96
	107	C	GLU	540	42.169	1.264	44.585	1.00	61.78
15	108	O	GLU	540	41.928	1.709	43.459	1.00	61.36
	109	N	PRO	541	41.214	0.713	45.352	1.00	63.77
	110	CD	PRO	541	41.365	0.053	46.659	1.00	58.98
20	111	CA	PRO	541	39.830	0.632	44.876	1.00	60.14
	112	CB	PRO	541	39.131	-0.149	45.988	1.00	59.62
	113	CG	PRO	541	39.978	0.122	47.195	1.00	60.56
25	114	C	PRO	541	39.180	1.991	44.592	1.00	62.36
	115	O	PRO	541	39.455	2.982	45.283	1.00	59.45
	116	N	GLU	542	38.332	2.039	43.563	1.00	60.43
30	117	CA	GLU	542	37.653	3.279	43.198	1.00	62.04
	118	CB	GLU	542	37.091	3.201	41.770	1.00	62.84
	119	CG	GLU	542	36.130	2.050	41.511	1.00	63.24
35	120	CD	GLU	542	35.745	1.911	40.031	1.00	63.39
	121	OE1	GLU	542	36.622	2.095	39.153	1.00	60.50
	122	OE2	GLU	542	34.568	1.599	39.743	1.00	59.31
40	123	C	GLU	542	36.548	3.515	44.208	1.00	63.11
	124	O	GLU	542	35.941	2.564	44.697	1.00	59.70
	125	N	VAL	543	36.304	4.783	44.528	1.00	61.53
45	126	CA	VAL	543	35.299	5.148	45.518	1.00	63.47
	127	CB	VAL	543	35.334	6.661	45.801	1.00	62.60
	128	CG1	VAL	543	34.467	6.984	46.987	1.00	60.93
50	129	CG2	VAL	543	36.762	7.103	46.064	1.00	59.59
	130	C	VAL	543	33.886	4.748	45.126	1.00	61.39
	131	O	VAL	543	33.495	4.877	43.965	1.00	60.79
55	132	N	LEU	544	33.128	4.267	46.109	1.00	62.56
	133	CA	LEU	544	31.759	3.836	45.882	1.00	60.63
	134	CB	LEU	544	31.501	2.486	46.547	1.00	63.18
55	135	CG	LEU	544	32.666	1.512	46.682	1.00	61.92
	136	CD1	LEU	544	33.702	2.114	47.638	1.00	62.67
	137	CD2	LEU	544	32.163	0.172	47.225	1.00	61.02
	138	C	LEU	544	30.754	4.844	46.423	1.00	58.48

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
139	O	LEU	544	31.097	5.715	47.225	1.00	59.01
140	N	TYR	545	29.508	4.698	45.974	1.00	60.35
141	CA	TYR	545	28.394	5.559	46.356	1.00	58.86
142	CB	TYR	545	27.616	5.977	45.105	1.00	59.62
143	CG	TYR	545	28.421	6.799	44.122	1.00	60.54
144	CD1	TYR	545	29.815	6.803	44.162	1.00	59.00
145	CE1	TYR	545	30.561	7.563	43.270	1.00	61.22
146	CD2	TYR	545	27.791	7.579	43.153	1.00	63.95
147	CE2	TYR	545	28.534	8.348	42.256	1.00	59.17
148	CZ	TYR	545	29.914	8.336	42.325	1.00	60.43
149	OH	TYR	545	30.654	9.120	41.478	1.00	60.96
150	C	TYR	545	27.501	4.743	47.269	1.00	64.48
151	O	TYR	545	27.449	3.517	47.151	1.00	60.43
152	N	ALA	546	26.789	5.415	48.168	1.00	62.22
153	CA	ALA	546	25.918	4.720	49.112	1.00	61.72
154	CB	ALA	546	25.780	5.540	50.378	1.00	60.83
155	C	ALA	546	24.536	4.377	48.570	1.00	61.54
156	O	ALA	546	23.886	3.461	49.065	1.00	58.65
157	N	GLY	547	24.089	5.100	47.549	1.00	60.89
158	CA	GLY	547	22.768	4.841	47.014	1.00	59.44
159	C	GLY	547	21.765	5.212	48.088	1.00	59.45
160	O	GLY	547	20.849	4.460	48.392	1.00	58.64
161	N	TYR	548	21.966	6.387	48.671	1.00	59.64
162	CA	TYR	548	21.119	6.921	49.733	1.00	61.47
163	CB	TYR	548	21.912	7.970	50.520	1.00	64.12
164	CG	TYR	548	21.244	8.421	51.783	1.00	58.90
165	CD1	TYR	548	21.049	7.534	52.833	1.00	61.61
166	CE1	TYR	548	20.414	7.927	53.992	1.00	63.67
167	CD2	TYR	548	20.785	9.726	51.926	1.00	60.05
168	CE2	TYR	548	20.144	10.129	53.084	1.00	60.57
169	CZ	TYR	548	19.964	9.218	54.112	1.00	64.94
170	OH	TYR	548	19.319	9.579	55.262	1.00	63.47
171	C	TYR	548	19.907	7.569	49.080	1.00	63.87
172	O	TYR	548	19.755	7.481	47.867	1.00	60.53
173	N	ASP	549	19.043	8.207	49.871	1.00	60.86
174	CA	ASP	549	17.881	8.882	49.307	1.00	62.83
175	CB	ASP	549	16.590	8.410	49.958	1.00	61.82

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	176	CG	ASP	549	15.487	8.213	48.935	1.00	59.25
	177	OD1	ASP	549	14.321	7.942	49.306	1.00	61.06
	178	OD2	ASP	549	15.810	8.328	47.734	1.00	61.75
10	179	C	ASP	549	17.979	10.402	49.411	1.00	62.83
	180	O	ASP	549	18.158	11.075	48.400	1.00	60.57
	181	N	SER	550	17.875	10.954	50.617	1.00	59.81
15	182	CA	SER	550	17.953	12.415	50.793	1.00	62.38
	183	CB	SER	550	19.325	12.951	50.386	1.00	56.99
	184	OG	SER	550	19.438	13.020	48.978	1.00	62.06
20	185	C	SER	550	16.894	13.126	49.957	1.00	62.44
	186	O	SER	550	16.893	14.350	49.843	1.00	61.89
	187	N	SER	551	16.018	12.343	49.343	1.00	61.48
25	188	CA	SER	551	14.924	12.875	48.557	1.00	60.05
	189	CB	SER	551	14.507	11.886	47.487	1.00	62.39
	190	OG	SER	551	13.838	10.800	48.100	1.00	61.65
30	191	C	SER	551	13.850	12.904	49.615	1.00	60.87
	192	O	SER	551	12.799	13.512	49.452	1.00	59.31
	193	N	VAL	552	14.142	12.200	50.703	1.00	61.91
35	194	CA	VAL	552	13.252	12.096	51.849	1.00	60.13
	195	CB	VAL	552	12.584	10.695	51.895	1.00	60.55
	196	CG1	VAL	552	11.242	10.744	51.187	1.00	59.77
40	197	CG2	VAL	552	13.461	9.674	51.211	1.00	62.73
	198	C	VAL	552	14.035	12.388	53.141	1.00	58.44
	199	O	VAL	552	15.269	12.482	53.116	1.00	60.59
45	200	N	PRO	553	13.326	12.571	54.278	1.00	59.91
	201	CD	PRO	553	11.861	12.614	54.440	1.00	61.19
	202	CA	PRO	553	13.974	12.859	55.559	1.00	59.95
50	203	CB	PRO	553	12.865	12.572	56.556	1.00	62.02
	204	CG	PRO	553	11.701	13.166	55.851	1.00	62.09
	205	C	PRO	553	15.263	12.093	55.839	1.00	62.80
55	206	O	PRO	553	15.525	11.035	55.259	1.00	61.14
	207	N	ASP	554	16.058	12.646	56.748	1.00	58.85
	208	CA	ASP	554	17.357	12.084	57.104	1.00	60.06
55	209	CB	ASP	554	18.462	13.098	56.755	1.00	61.56
	210	CG	ASP	554	18.836	13.106	55.280	1.00	62.42
	211	OD1	ASP	554	17.961	12.964	54.390	1.00	59.77
	212	OD2	ASP	554	20.038	13.286	55.014	1.00	59.95

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
213	C	ASP	554	17.535	11.703	58.575	1.00	56.92
214	O	ASP	554	18.402	12.273	59.229	1.00	61.20
215	N	SER	555	16.767	10.761	59.116	1.00	62.60
216	CA	SER	555	16.970	10.398	60.526	1.00	63.72
217	CB	SER	555	15.998	9.296	60.948	1.00	63.32
218	OG	SER	555	16.267	8.089	60.255	1.00	60.75
219	C	SER	555	18.404	9.905	60.749	1.00	61.32
220	O	SER	555	19.093	9.556	59.794	1.00	59.49
221	N	THR	556	18.855	9.877	62.002	1.00	63.20
222	CA	THR	556	20.211	9.407	62.308	1.00	62.68
223	CB	THR	556	20.554	9.487	63.826	1.00	62.64
224	OG1	THR	556	20.893	10.831	64.183	1.00	62.26
225	CG2	THR	556	21.739	8.582	64.158	1.00	62.40
226	C	THR	556	20.387	7.955	61.902	1.00	62.17
227	O	THR	556	21.196	7.633	61.030	1.00	63.77
228	N	TRP	557	19.624	7.082	62.554	1.00	63.04
229	CA	TRP	557	19.696	5.652	62.294	1.00	60.39
230	CB	TRP	557	18.505	4.923	62.964	1.00	61.26
231	CG	TRP	557	17.324	4.805	62.064	1.00	64.02
232	CD2	TRP	557	17.074	3.747	61.123	1.00	60.71
233	CE2	TRP	557	15.970	4.142	60.332	1.00	58.32
234	CE3	TRP	557	17.684	2.511	60.865	1.00	62.45
235	CD1	TRP	557	16.378	5.760	61.825	1.00	60.50
236	NE1	TRP	557	15.562	5.373	60.780	1.00	59.73
237	CZ2	TRP	557	15.464	3.341	59.296	1.00	61.79
238	CZ3	TRP	557	17.184	1.716	59.836	1.00	62.55
239	CH2	TRP	557	16.084	2.136	59.065	1.00	57.76
240	C	TRP	557	19.731	5.362	60.783	1.00	61.95
241	O	TRP	557	20.479	4.493	60.332	1.00	59.61
242	N	ARG	558	18.946	6.099	60.001	1.00	61.85
243	CA	ARG	558	18.898	5.873	58.555	1.00	64.57
244	CB	ARG	558	17.744	6.651	57.926	1.00	59.03
245	CG	ARG	558	17.303	6.107	56.582	1.00	62.63
246	CD	ARG	558	16.012	6.780	56.133	1.00	59.07
247	NE	ARG	558	16.221	7.958	55.288	1.00	61.76
248	CZ	ARG	558	16.594	7.911	54.011	1.00	63.52
249	NH1	ARG	558	16.805	6.745	53.420	1.00	63.08

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	250	NH2	ARG	558	16.750	9.031	53.319	1.00	60.97
	251	C	ARG	558	20.200	6.222	57.841	1.00	64.20
	252	O	ARG	558	20.573	5.566	56.869	1.00	65.47
10	253	N	ILE	559	20.877	7.266	58.307	1.00	62.87
	254	CA	ILE	559	22.156	7.678	57.726	1.00	59.66
	255	CB	ILE	559	22.639	9.040	58.329	1.00	62.98
15	256	CG2	ILE	559	24.101	9.278	57.993	1.00	59.64
	257	CG1	ILE	559	21.794	10.196	57.791	1.00	61.72
	258	CD1	ILE	559	22.091	10.556	56.351	1.00	60.58
20	259	C	ILE	559	23.152	6.585	58.119	1.00	62.05
	260	O	ILE	559	23.838	5.995	57.274	1.00	61.48
	261	N	MET	560	23.188	6.332	59.425	1.00	60.47
25	262	CA	MET	560	24.056	5.340	60.036	1.00	59.72
	263	CB	MET	560	23.799	5.286	61.554	1.00	61.50
	264	CG	MET	560	24.863	6.016	62.358	1.00	59.68
30	265	SD	MET	560	24.765	5.946	64.183	1.00	62.00
	266	CE	MET	560	25.827	7.029	64.314	1.00	56.75
	267	C	MET	560	23.910	3.950	59.421	1.00	63.13
35	268	O	MET	560	24.908	3.299	59.122	1.00	60.43
	269	N	THR	561	22.680	3.493	59.215	1.00	59.86
	270	CA	THR	561	22.487	2.183	58.619	1.00	62.03
40	271	CB	THR	561	21.005	1.771	58.603	1.00	60.73
	272	OG1	THR	561	20.483	1.777	59.938	1.00	58.44
	273	CG2	THR	561	20.862	0.370	58.025	1.00	59.27
45	274	C	THR	561	23.005	2.192	57.190	1.00	62.25
	275	O	THR	561	23.565	1.211	56.724	1.00	59.53
	276	N	THR	562	22.813	3.296	56.482	1.00	61.35
50	277	CA	THR	562	23.305	3.365	55.112	1.00	62.18
	278	CB	THR	562	22.728	4.593	54.342	1.00	58.86
	279	OG1	THR	562	21.338	4.375	54.051	1.00	58.36
55	280	CG2	THR	562	23.473	4.805	53.033	1.00	58.66
	281	C	THR	562	24.830	3.432	55.157	1.00	62.40
	282	O	THR	562	25.509	3.011	54.225	1.00	59.62
55	283	N	LEU	563	25.374	3.949	56.252	1.00	60.06
	284	CA	LEU	563	26.825	4.026	56.382	1.00	61.98
	285	CB	LEU	563	27.230	5.045	57.451	1.00	59.10
	286	CG	LEU	563	27.004	6.519	57.119	1.00	62.03

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
287	CD1	LEU	563	27.667	7.377	58.180	1.00	59.83
288	CD2	LEU	563	27.574	6.827	55.745	1.00	63.51
289	C	LEU	563	27.406	2.657	56.730	1.00	63.21
290	O	LEU	563	28.592	2.410	56.529	1.00	59.14
291	N	ASN	564	26.567	1.773	57.264	1.00	59.68
292	CA	ASN	564	27.001	0.427	57.606	1.00	62.50
293	CB	ASN	564	26.110	-0.166	58.689	1.00	61.63
294	CG	ASN	564	26.456	0.349	60.058	1.00	62.37
295	OD1	ASN	564	27.625	0.513	60.381	1.00	62.36
296	ND2	ASN	564	25.447	0.590	60.881	1.00	59.03
297	C	ASN	564	26.949	-0.442	56.356	1.00	61.40
298	O	ASN	564	27.823	-1.266	56.121	1.00	61.63
299	N	MET	565	25.923	-0.251	55.543	1.00	62.42
300	CA	MET	565	25.804	-1.022	54.320	1.00	63.45
301	CB	MET	565	24.483	-0.701	53.632	1.00	59.10
302	CG	MET	565	23.266	-0.999	54.488	1.00	62.52
303	SD	MET	565	23.154	-2.742	54.883	1.00	63.35
304	CE	MET	565	22.918	-2.702	56.627	1.00	60.16
305	C	MET	565	26.967	-0.669	53.410	1.00	62.27
306	O	MET	565	27.475	-1.509	52.677	1.00	62.01
307	N	LEU	566	27.382	0.590	53.462	1.00	62.25
308	CA	LEU	566	28.495	1.064	52.656	1.00	60.20
309	CB	LEU	566	28.596	2.594	52.741	1.00	59.50
310	CG	LEU	566	29.801	3.267	52.076	1.00	64.18
311	CD1	LEU	566	29.685	3.195	50.565	1.00	61.46
312	CD2	LEU	566	29.869	4.700	52.516	1.00	62.10
313	C	LEU	566	29.756	0.424	53.218	1.00	62.85
314	O	LEU	566	30.576	-0.116	52.474	1.00	60.20
315	N	GLY	567	29.886	0.477	54.542	1.00	59.45
316	CA	GLY	567	31.040	-0.095	55.207	1.00	59.94
317	C	GLY	567	31.316	-1.516	54.768	1.00	60.71
318	O	GLY	567	32.461	-1.890	54.520	1.00	59.79
319	N	GLY	568	30.261	-2.310	54.667	1.00	61.99
320	CA	GLY	568	30.417	-3.687	54.254	1.00	59.73
321	C	GLY	568	31.050	-3.836	52.888	1.00	60.65
322	O	GLY	568	32.008	-4.590	52.724	1.00	63.15
323	N	ARG	569	30.529	-3.112	51.907	1.00	58.99

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	324	CA	ARG	569	31.049	-3.208	50.557	1.00	60.81
	325	CB	ARG	569	30.109	-2.483	49.600	1.00	60.57
	326	CG	ARG	569	28.696	-3.029	49.701	1.00	61.60
10	327	CD	ARG	569	27.806	-2.602	48.556	1.00	64.73
	328	NE	ARG	569	27.561	-1.168	48.564	1.00	61.17
	329	CZ	ARG	569	27.939	-0.352	47.590	1.00	60.00
15	330	NH1	ARG	569	28.577	-0.841	46.532	1.00	60.46
	331	NH2	ARG	569	27.681	0.946	47.680	1.00	63.69
	332	C	ARG	569	32.462	-2.676	50.447	1.00	61.15
20	333	O	ARG	569	33.249	-3.137	49.620	1.00	60.59
	334	N	GLN	570	32.788	-1.713	51.295	1.00	60.73
	335	CA	GLN	570	34.123	-1.132	51.300	1.00	62.31
25	336	CB	GLN	570	34.143	0.150	52.120	1.00	59.04
	337	CG	GLN	570	33.608	1.361	51.417	1.00	62.03
	338	CD	GLN	570	33.782	2.606	52.247	1.00	56.35
30	339	OE1	GLN	570	33.460	3.698	51.801	1.00	62.86
	340	NE2	GLN	570	34.295	2.449	53.467	1.00	63.17
	341	C	GLN	570	35.144	-2.093	51.882	1.00	61.15
35	342	O	GLN	570	36.293	-2.134	51.441	1.00	60.50
	343	N	VAL	571	34.732	-2.837	52.903	1.00	60.99
	344	CA	VAL	571	35.615	-3.792	53.554	1.00	61.91
40	345	CB	VAL	571	35.054	-4.200	54.930	1.00	58.42
	346	CG1	VAL	571	35.822	-5.393	55.485	1.00	61.27
	347	CG2	VAL	571	35.160	-3.007	55.891	1.00	60.58
45	348	C	VAL	571	35.805	-5.007	52.665	1.00	62.66
	349	O	VAL	571	36.698	-5.820	52.885	1.00	58.99
	350	N	ILE	572	34.958	-5.116	51.652	1.00	63.61
50	351	CA	ILE	572	35.042	-6.206	50.695	1.00	63.76
	352	CB	ILE	572	33.649	-6.539	50.103	1.00	60.98
	353	CG2	ILE	572	33.794	-7.443	48.883	1.00	63.63
55	354	CG1	ILE	572	32.782	-7.192	51.183	1.00	61.03
	355	CD1	ILE	572	31.346	-7.366	50.801	1.00	62.17
	356	C	ILE	572	35.999	-5.772	49.589	1.00	60.35
55	357	O	ILE	572	36.733	-6.587	49.042	1.00	62.13
	358	N	ALA	573	35.984	-4.481	49.265	1.00	62.76
	359	CA	ALA	573	36.879	-3.936	48.251	1.00	58.47
	360	CB	ALA	573	36.502	-2.496	47.940	1.00	61.48

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
361	C	ALA	573	38.271	-3.997	48.872	1.00	61.14
362	O	ALA	573	39.294	-4.088	48.180	1.00	60.46
363	N	ALA	574	38.273	-3.964	50.200	1.00	60.84
364	CA	ALA	574	39.477	-4.008	51.003	1.00	61.42
365	CB	ALA	574	39.098	-3.888	52.465	1.00	60.18
366	C	ALA	574	40.294	-5.282	50.771	1.00	58.96
367	O	ALA	574	41.506	-5.217	50.518	1.00	61.38
368	N	VAL	575	39.631	-6.435	50.861	1.00	59.99
369	CA	VAL	575	40.296	-7.720	50.664	1.00	59.60
370	CB	VAL	575	39.309	-8.898	50.732	1.00	56.06
371	CG1	VAL	575	40.070	-10.197	50.570	1.00	62.55
372	CG2	VAL	575	38.547	-8.880	52.057	1.00	63.34
373	C	VAL	575	41.009	-7.779	49.318	1.00	60.96
374	O	VAL	575	42.222	-7.981	49.264	1.00	62.47
375	N	LYS	576	40.265	-7.584	48.236	1.00	59.97
376	CA	LYS	576	40.851	-7.628	46.901	1.00	62.25
377	CB	LYS	576	39.770	-7.391	45.860	1.00	60.99
378	CG	LYS	576	40.115	-7.866	44.462	1.00	61.35
379	CD	LYS	576	38.905	-7.708	43.568	1.00	63.13
380	CE	LYS	576	37.667	-8.234	44.276	1.00	62.07
381	NZ	LYS	576	36.420	-7.912	43.531	1.00	59.76
382	C	LYS	576	41.957	-6.593	46.742	1.00	63.69
383	O	LYS	576	42.673	-6.573	45.742	1.00	59.32
384	N	TRP	577	42.074	-5.723	47.734	1.00	62.59
385	CA	TRP	577	43.091	-4.694	47.734	1.00	62.15
386	CB	TRP	577	42.556	-3.432	48.424	1.00	60.50
387	CG	TRP	577	43.620	-2.458	48.780	1.00	63.03
388	CD2	TRP	577	44.140	-2.200	50.090	1.00	58.79
389	CE2	TRP	577	45.189	-1.272	49.945	1.00	64.04
390	CE3	TRP	577	43.824	-2.668	51.372	1.00	60.56
391	CD1	TRP	577	44.346	-1.698	47.924	1.00	62.09
392	NE1	TRP	577	45.293	-0.983	48.611	1.00	61.93
393	CZ2	TRP	577	45.930	-0.798	51.032	1.00	61.40
394	CZ3	TRP	577	44.566	-2.197	52.458	1.00	59.59
395	CH2	TRP	577	45.607	-1.271	52.277	1.00	61.92
396	C	TRP	577	44.263	-5.272	48.509	1.00	64.09
397	O	TRP	577	45.403	-5.238	48.055	1.00	61.89

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
398	N	ALA	578	43.958	-5.824	49.678	1.00	60.10
399	CA	ALA	578	44.974	-6.411	50.541	1.00	61.99
400	CB	ALA	578	44.342	-6.937	51.828	1.00	57.97
401	C	ALA	578	45.704	-7.526	49.828	1.00	61.84
402	O	ALA	578	46.890	-7.718	50.034	1.00	60.47
403	N	LYS	579	44.988	-8.251	48.979	1.00	61.79
404	CA	LYS	579	45.573	-9.354	48.233	1.00	60.65
405	CB	LYS	579	44.472	-10.320	47.784	1.00	62.20
406	CG	LYS	579	43.479	-10.656	48.893	1.00	63.14
407	CD	LYS	579	42.688	-11.944	48.636	1.00	58.27
408	CE	LYS	579	41.775	-11.862	47.419	1.00	58.47
409	NZ	LYS	579	41.093	-13.167	47.129	1.00	62.99
410	C	LYS	579	46.389	-8.895	47.024	1.00	61.02
411	O	LYS	579	47.014	-9.713	46.356	1.00	63.16
412	N	ALA	580	46.383	-7.596	46.738	1.00	61.84
413	CA	ALA	580	47.153	-7.079	45.610	1.00	58.94
414	CB	ALA	580	46.339	-6.062	44.817	1.00	61.14
415	C	ALA	580	48.439	-6.446	46.137	1.00	60.40
416	O	ALA	580	49.378	-6.190	45.374	1.00	60.45
417	N	ILE	581	48.465	-6.197	47.445	1.00	60.82
418	CA	ILE	581	49.631	-5.631	48.111	1.00	60.29
419	CB	ILE	581	49.375	-5.412	49.630	1.00	58.24
420	CG2	ILE	581	50.654	-4.997	50.324	1.00	63.40
421	CG1	ILE	581	48.295	-4.353	49.847	1.00	62.12
422	CD1	ILE	581	47.769	-4.324	51.257	1.00	62.13
423	C	ILE	581	50.690	-6.706	47.965	1.00	62.02
424	O	ILE	581	50.541	-7.805	48.500	1.00	61.29
425	N	PRO	582	51.773	-6.412	47.233	1.00	62.24
426	CD	PRO	582	52.137	-5.123	46.623	1.00	61.16
427	CA	PRO	582	52.837	-7.397	47.041	1.00	64.30
428	CB	PRO	582	53.983	-6.563	46.486	1.00	61.32
429	CG	PRO	582	53.294	-5.515	45.720	1.00	57.84
430	C	PRO	582	53.208	-8.082	48.341	1.00	62.26
431	O	PRO	582	53.291	-7.451	49.390	1.00	61.55
432	N	GLY	583	53.413	-9.386	48.268	1.00	60.04
433	CA	GLY	583	53.788	-10.138	49.447	1.00	63.24
434	C	GLY	583	52.721	-10.313	50.509	1.00	58.28

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5 435	O	GLY	583	52.976	-10.962	51.519	1.00	61.03
436	N	PHE	584	51.527	-9.758	50.320	1.00	59.53
437	CA	PHE	584	50.517	-9.932	51.354	1.00	60.33
10 438	CB	PHE	584	49.356	-8.960	51.200	1.00	59.83
439	CG	PHE	584	48.314	-9.107	52.276	1.00	62.69
440	CD1	PHE	584	48.583	-8.699	53.576	1.00	65.80
441	CD2	PHE	584	47.075	-9.677	52.000	1.00	59.15
15 442	CE1	PHE	584	47.636	-8.854	54.586	1.00	63.90
443	CE2	PHE	584	46.123	-9.837	53.000	1.00	62.77
444	CZ	PHE	584	46.405	-9.423	54.296	1.00	62.23
20 445	C	PHE	584	49.960	-11.336	51.359	1.00	59.87
446	O	PHE	584	49.874	-11.967	52.415	1.00	60.23
447	N	ARG	585	49.584	-11.848	50.193	1.00	61.22
448	CA	ARG	585	49.021	-13.183	50.207	1.00	62.87
25 449	CB	ARG	585	48.025	-13.405	49.042	1.00	61.05
450	CG	ARG	585	48.486	-13.212	47.602	1.00	62.14
451	CD	ARG	585	47.253	-13.326	46.690	1.00	59.51
30 452	NE	ARG	585	46.321	-14.325	47.226	1.00	57.83
453	CZ	ARG	585	45.253	-14.826	46.592	1.00	62.40
454	NH1	ARG	585	44.934	-14.430	45.360	1.00	64.51
455	NH2	ARG	585	44.509	-15.752	47.194	1.00	62.15
35 456	C	ARG	585	50.053	-14.290	50.303	1.00	61.04
457	O	ARG	585	49.781	-15.436	49.962	1.00	59.18
458	N	ASN	586	51.232	-13.935	50.811	1.00	59.32
40 459	CA	ASN	586	52.319	-14.893	51.021	1.00	62.11
460	CB	ASN	586	53.659	-14.329	50.545	1.00	57.88
461	CG	ASN	586	53.910	-14.596	49.071	1.00	62.73
462	OD1	ASN	586	54.772	-13.964	48.450	1.00	64.87
45 463	ND2	ASN	586	53.164	-15.551	48.504	1.00	63.32
464	C	ASN	586	52.396	-15.218	52.503	1.00	61.24
465	O	ASN	586	53.093	-16.138	52.916	1.00	62.45
50 466	N	LEU	587	51.692	-14.446	53.314	1.00	62.98
467	CA	LEU	587	51.677	-14.732	54.735	1.00	63.89
468	CB	LEU	587	51.210	-13.502	55.522	1.00	63.58
469	CG	LEU	587	52.163	-12.299	55.501	1.00	63.59
55 470	CD1	LEU	587	51.405	-11.009	55.348	1.00	58.78
471	CD2	LEU	587	52.967	-12.280	56.773	1.00	60.86

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	472	C	LEU	587	50.679	-15.879	54.848	1.00	61.92
	473	O	LEU	587	50.000	-16.209	53.865	1.00	61.57
	474	N	HIS	588	50.598	-16.497	56.024	1.00	57.84
10	475	CA	HIS	588	49.676	-17.609	56.235	1.00	62.30
	476	CB	HIS	588	49.674	-18.016	57.710	1.00	63.47
	477	CG	HIS	588	49.180	-19.411	57.962	1.00	62.99
15	478	CD2	HIS	588	49.817	-20.502	58.447	1.00	58.47
	479	ND1	HIS	588	47.886	-19.808	57.705	1.00	57.63
	480	CE1	HIS	588	47.748	-21.083	58.021	1.00	60.07
20	481	NE2	HIS	588	48.905	-21.527	58.474	1.00	61.65
	482	C	HIS	588	48.304	-17.100	55.839	1.00	61.24
	483	O	HIS	588	48.137	-15.900	55.641	1.00	58.81
25	484	N	LEU	589	47.325	-17.990	55.714	1.00	60.37
	485	CA	LEU	589	45.990	-17.542	55.346	1.00	63.23
	486	CB	LEU	589	45.219	-18.626	54.588	1.00	60.24
30	487	CG	LEU	589	44.233	-18.127	53.516	1.00	59.80
	488	CD1	LEU	589	43.798	-19.286	52.630	1.00	65.35
	489	CD2	LEU	589	43.025	-17.486	54.148	1.00	61.31
35	490	C	LEU	589	45.249	-17.184	56.616	1.00	59.85
	491	O	LEU	589	44.150	-16.645	56.563	1.00	59.20
	492	N	ASP	590	45.852	-17.469	57.763	1.00	60.93
40	493	CA	ASP	590	45.200	-17.158	59.027	1.00	61.82
	494	CB	ASP	590	45.551	-18.204	60.097	1.00	62.69
	495	CG	ASP	590	44.823	-19.529	59.898	1.00	58.29
45	496	OD1	ASP	590	44.642	-19.955	58.738	1.00	59.06
	497	OD2	ASP	590	44.447	-20.159	60.910	1.00	64.34
	498	C	ASP	590	45.608	-15.771	59.504	1.00	59.77
50	499	O	ASP	590	44.915	-15.153	60.314	1.00	60.73
	500	N	ASP	591	46.734	-15.278	59.001	1.00	59.62
	501	CA	ASP	591	47.211	-13.960	59.401	1.00	61.48
55	502	CB	ASP	591	48.733	-13.861	59.240	1.00	60.79
	503	CG	ASP	591	49.479	-14.900	60.065	1.00	57.79
	504	OD1	ASP	591	49.012	-15.239	61.176	1.00	66.77
55	505	OD2	ASP	591	50.543	-15.366	59.606	1.00	65.51
	506	C	ASP	591	46.531	-12.927	58.529	1.00	62.56
	507	O	ASP	591	46.255	-11.812	58.967	1.00	59.26
	508	N	GLN	592	46.278	-13.323	57.285	1.00	62.10

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
509	CA	GLN	592	45.613	-12.473	56.316	1.00	61.30
510	CB	GLN	592	45.432	-13.227	54.998	1.00	62.26
511	CG	GLN	592	46.751	-13.456	54.277	1.00	60.59
512	CD	GLN	592	46.595	-14.100	52.909	1.00	59.32
513	OE1	GLN	592	45.597	-13.887	52.213	1.00	62.27
514	NE2	GLN	592	47.600	-14.875	52.505	1.00	62.12
515	C	GLN	592	44.269	-12.097	56.906	1.00	64.75
516	O	GLN	592	43.768	-10.993	56.706	1.00	62.08
517	N	MET	593	43.701	-13.028	57.660	1.00	59.14
518	CA	MET	593	42.413	-12.815	58.302	1.00	61.78
519	CB	MET	593	41.740	-14.162	58.597	1.00	58.91
520	CG	MET	593	41.290	-14.935	57.357	1.00	64.30
521	SD	MET	593	40.510	-16.524	57.776	1.00	58.06
522	CE	MET	593	39.514	-16.029	59.273	1.00	61.88
523	C	MET	593	42.571	-12.014	59.594	1.00	61.38
524	O	MET	593	41.802	-11.089	59.837	1.00	60.42
525	N	THR	594	43.565	-12.361	60.415	1.00	61.83
526	CA	THR	594	43.781	-11.648	61.674	1.00	61.88
527	CB	THR	594	44.924	-12.267	62.518	1.00	57.74
528	OG1	THR	594	45.252	-13.571	62.023	1.00	65.18
529	CG2	THR	594	44.489	-12.393	63.977	1.00	62.23
530	C	THR	594	44.127	-10.194	61.378	1.00	62.61
531	O	THR	594	43.673	-9.279	62.071	1.00	60.17
532	N	LEU	595	44.927	-9.987	60.337	1.00	60.31
533	CA	LEU	595	45.325	-8.647	59.938	1.00	61.48
534	CB	LEU	595	46.372	-8.712	58.826	1.00	62.70
535	CG	LEU	595	47.788	-9.074	59.266	1.00	60.61
536	CD1	LEU	595	48.711	-9.054	58.067	1.00	63.20
537	CD2	LEU	595	48.268	-8.083	60.316	1.00	62.58
538	C	LEU	595	44.128	-7.823	59.475	1.00	63.38
539	O	LEU	595	43.835	-6.779	60.051	1.00	60.70
540	N	LEU	596	43.439	-8.290	58.436	1.00	60.66
541	CA	LEU	596	42.282	-7.571	57.924	1.00	60.47
542	CB	LEU	596	41.703	-8.278	56.699	1.00	60.10
543	CG	LEU	596	42.351	-7.811	55.392	1.00	60.73
544	CD1	LEU	596	42.036	-8.767	54.254	1.00	59.40
545	CD2	LEU	596	41.859	-6.407	55.073	1.00	62.48

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
546	C	LEU	596	41.223	-7.424	58.989	1.00	58.32
547	O	LEU	596	40.451	-6.480	58.965	1.00	61.48
548	N	GLN	597	41.201	-8.354	59.935	1.00	62.48
549	CA	GLN	597	40.230	-8.327	61.031	1.00	64.28
550	CB	GLN	597	40.128	-9.712	61.685	1.00	59.49
551	CG	GLN	597	38.936	-10.561	61.279	1.00	64.66
552	CD	GLN	597	38.972	-11.940	61.920	1.00	60.50
553	OE1	GLN	597	39.080	-12.078	63.149	1.00	60.07
554	NE2	GLN	597	38.881	-12.975	61.087	1.00	65.01
555	C	GLN	597	40.612	-7.314	62.110	1.00	61.61
556	O	GLN	597	39.780	-6.933	62.932	1.00	61.06
557	N	TYR	598	41.875	-6.896	62.097	1.00	64.61
558	CA	TYR	598	42.418	-5.958	63.075	1.00	60.76
559	CB	TYR	598	43.761	-6.468	63.588	1.00	59.35
560	CG	TYR	598	43.692	-7.564	64.613	1.00	63.67
561	CD1	TYR	598	42.509	-8.257	64.850	1.00	61.84
562	CE1	TYR	598	42.451	-9.262	65.812	1.00	61.13
563	CD2	TYR	598	44.820	-7.906	65.358	1.00	61.13
564	CE2	TYR	598	44.774	-8.915	66.322	1.00	62.04
565	CZ	TYR	598	43.588	-9.583	66.544	1.00	60.04
566	OH	TYR	598	43.536	-10.549	67.519	1.00	62.57
567	C	TYR	598	42.639	-4.553	62.549	1.00	62.24
568	O	TYR	598	43.158	-3.690	63.256	1.00	61.45
569	N	SER	599	42.278	-4.312	61.305	1.00	58.28
570	CA	SER	599	42.491	-2.988	60.774	1.00	62.69
571	CB	SER	599	43.837	-2.949	60.046	1.00	62.55
572	OG	SER	599	44.008	-4.083	59.216	1.00	62.72
573	C	SER	599	41.365	-2.525	59.867	1.00	64.40
574	O	SER	599	41.398	-1.405	59.367	1.00	62.40
575	N	TRP	600	40.358	-3.375	59.677	1.00	59.48
576	CA	TRP	600	39.245	-3.026	58.807	1.00	62.88
577	CB	TRP	600	38.073	-4.031	58.932	1.00	64.17
578	CG	TRP	600	37.282	-3.951	60.198	1.00	62.02
579	CD2	TRP	600	36.105	-3.166	60.420	1.00	58.67
580	CE2	TRP	600	35.754	-3.311	61.781	1.00	61.68
581	CE3	TRP	600	35.314	-2.350	59.603	1.00	62.68
582	CD1	TRP	600	37.583	-4.533	61.395	1.00	58.92

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
583	NE1	TRP	600	36.672	-4.151	62.355	1.00	64.28
584	CZ2	TRP	600	34.648	-2.666	62.342	1.00	61.17
585	CZ3	TRP	600	34.217	-1.711	60.159	1.00	58.94
586	CH2	TRP	600	33.894	-1.871	61.516	1.00	61.08
587	C	TRP	600	38.789	-1.630	59.169	1.00	62.61
588	O	TRP	600	38.533	-0.805	58.308	1.00	62.45
589	N	MET	601	38.744	-1.344	60.458	1.00	63.90
590	CA	MET	601	38.298	-0.049	60.884	1.00	60.96
591	CB	MET	601	37.968	-0.064	62.351	1.00	60.46
592	CG	MET	601	37.139	1.112	62.702	1.00	61.28
593	SD	MET	601	35.774	1.420	61.631	1.00	59.33
594	CE	MET	601	34.684	1.638	62.889	1.00	64.63
595	C	MET	601	39.225	1.129	60.577	1.00	61.08
596	O	MET	601	38.758	2.167	60.114	1.00	60.27
597	N	SER	602	40.521	0.979	60.854	1.00	61.23
598	CA	SER	602	41.488	2.035	60.581	1.00	59.98
599	CB	SER	602	42.872	1.647	61.083	1.00	60.99
600	OG	SER	602	42.783	1.022	62.350	1.00	66.17
601	C	SER	602	41.536	2.214	59.079	1.00	60.99
602	O	SER	602	41.609	3.327	58.581	1.00	64.11
603	N	LEU	603	41.494	1.108	58.351	1.00	59.44
604	CA	LEU	603	41.522	1.185	56.901	1.00	61.46
605	CB	LEU	603	41.402	-0.212	56.280	1.00	59.31
606	CG	LEU	603	42.646	-1.097	56.346	1.00	61.54
607	CD1	LEU	603	42.415	-2.362	55.549	1.00	63.99
608	CD2	LEU	603	43.828	-0.346	55.787	1.00	63.36
609	C	LEU	603	40.386	2.061	56.408	1.00	60.47
610	O	LEU	603	40.599	3.062	55.731	1.00	63.39
611	N	MET	604	39.173	1.688	56.784	1.00	63.54
612	CA	MET	604	38.000	2.417	56.365	1.00	62.81
613	CB	MET	604	36.770	1.623	56.723	1.00	58.90
614	CG	MET	604	36.632	0.429	55.842	1.00	59.86
615	SD	MET	604	37.633	0.438	54.374	1.00	62.53
616	CE	MET	604	36.663	-0.510	53.559	1.00	60.72
617	C	MET	604	37.898	3.832	56.856	1.00	60.43
618	O	MET	604	37.397	4.695	56.132	1.00	62.37
619	N	ALA	605	38.375	4.076	58.072	1.00	59.95

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	620	CA	ALA	605	38.357	5.409	58.664	1.00	60.49
	621	CB	ALA	605	38.667	5.317	60.132	1.00	59.15
	622	C	ALA	605	39.381	6.309	57.985	1.00	61.50
10	623	O	ALA	605	39.071	7.427	57.583	1.00	59.82
	624	N	PHE	606	40.608	5.810	57.870	1.00	63.59
	625	CA	PHE	606	41.700	6.554	57.258	1.00	60.15
15	626	CB	PHE	606	42.981	5.713	57.285	1.00	63.75
	627	CG	PHE	606	44.237	6.490	56.999	1.00	64.30
	628	CD1	PHE	606	44.723	7.424	57.913	1.00	61.77
20	629	CD2	PHE	606	44.957	6.265	55.829	1.00	60.74
	630	CE1	PHE	606	45.910	8.118	57.665	1.00	64.00
	631	CE2	PHE	606	46.145	6.955	55.575	1.00	62.47
25	632	CZ	PHE	606	46.620	7.879	56.496	1.00	63.95
	633	C	PHE	606	41.362	6.933	55.825	1.00	61.96
	634	O	PHE	606	41.751	7.991	55.356	1.00	60.07
30	635	N	ALA	607	40.644	6.063	55.126	1.00	62.00
	636	CA	ALA	607	40.264	6.338	53.745	1.00	57.50
	637	CB	ALA	607	39.888	5.051	53.039	1.00	59.69
35	638	C	ALA	607	39.105	7.324	53.684	1.00	64.88
	639	O	ALA	607	38.931	8.030	52.703	1.00	59.60
	640	N	LEU	608	38.292	7.361	54.723	1.00	59.93
40	641	CA	LEU	608	37.196	8.307	54.725	1.00	61.70
	642	CB	LEU	608	36.222	7.972	55.883	1.00	59.57
	643	CG	LEU	608	35.125	8.918	56.402	1.00	62.57
45	644	CD1	LEU	608	34.229	9.360	55.287	1.00	63.51
	645	CD2	LEU	608	34.298	8.246	57.488	1.00	59.98
	646	C	LEU	608	37.862	9.662	54.935	1.00	61.71
50	647	O	LEU	608	37.500	10.645	54.294	1.00	57.56
	648	N	GLY	609	38.869	9.692	55.806	1.00	59.60
	649	CA	GLY	609	39.583	10.920	56.086	1.00	60.49
55	650	C	GLY	609	40.232	11.505	54.850	1.00	59.17
	651	O	GLY	609	40.189	12.710	54.625	1.00	61.65
	652	N	TRP	610	40.835	10.650	54.039	1.00	62.47
60	653	CA	TRP	610	41.488	11.102	52.823	1.00	61.40
	654	CB	TRP	610	42.141	9.917	52.123	1.00	62.68
	655	CG	TRP	610	42.744	10.264	50.817	1.00	62.61
65	656	CD2	TRP	610	43.955	10.991	50.604	1.00	61.10

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	657	CE2	TRP	610	44.139	11.095	49.209	1.00	62.45
	658	CE3	TRP	610	44.906	11.565	51.457	1.00	63.78
	659	CD1	TRP	610	42.254	9.965	49.582	1.00	58.08
10	660	NE1	TRP	610	43.086	10.459	48.608	1.00	62.17
	661	CZ2	TRP	610	45.238	11.751	48.646	1.00	60.53
	662	CZ3	TRP	610	46.001	12.219	50.896	1.00	62.27
	663	CH2	TRP	610	46.156	12.305	49.505	1.00	60.31
15	664	C	TRP	610	40.517	11.797	51.874	1.00	60.80
	665	O	TRP	610	40.797	12.866	51.358	1.00	60.72
	666	N	ARG	611	39.368	11.191	51.639	1.00	61.36
20	667	CA	ARG	611	38.412	11.790	50.738	1.00	58.33
	668	CB	ARG	611	37.254	10.817	50.486	1.00	62.33
	669	CG	ARG	611	37.684	9.490	49.873	1.00	60.18
	670	CD	ARG	611	36.476	8.686	49.426	1.00	59.83
25	671	NE	ARG	611	35.604	8.333	50.544	1.00	61.17
	672	CZ	ARG	611	35.817	7.308	51.366	1.00	59.54
	673	NH1	ARG	611	36.875	6.528	51.187	1.00	61.47
30	674	NH2	ARG	611	34.988	7.072	52.376	1.00	62.25
	675	C	ARG	611	37.898	13.128	51.277	1.00	62.93
	676	O	ARG	611	37.610	14.051	50.502	1.00	61.13
	677	N	SER	612	37.806	13.234	52.603	1.00	60.26
35	678	CA	SER	612	37.321	14.450	53.263	1.00	63.90
	679	CB	SER	612	37.057	14.172	54.736	1.00	62.00
	680	OG	SER	612	36.011	13.234	54.875	1.00	59.62
40	681	C	SER	612	38.263	15.637	53.137	1.00	61.68
	682	O	SER	612	37.831	16.776	52.975	1.00	59.32
	683	N	TYR	613	39.552	15.352	53.226	1.00	64.48
45	684	CA	TYR	613	40.600	16.351	53.111	1.00	60.97
	685	CB	TYR	613	41.920	15.725	53.587	1.00	56.65
	686	CG	TYR	613	43.169	16.122	52.830	1.00	60.73
	687	CD1	TYR	613	43.569	17.456	52.746	1.00	64.60
50	688	CE1	TYR	613	44.737	17.812	52.086	1.00	60.79
	689	CD2	TYR	613	43.971	15.153	52.229	1.00	61.29
	690	CE2	TYR	613	45.142	15.500	51.564	1.00	63.40
55	691	CZ	TYR	613	45.522	16.830	51.497	1.00	61.75
	692	OH	TYR	613	46.690	17.173	50.854	1.00	62.46
	693	C	TYR	613	40.712	16.822	51.667	1.00	62.41

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	694	O	TYR	613	40.954	17.996	51.395	1.00	61.34
	695	N	ARG	614	40.511	15.896	50.745	1.00	61.73
	696	CA	ARG	614	40.623	16.190	49.328	1.00	61.64
10	697	CB	ARG	614	40.835	14.880	48.545	1.00	62.80
	698	CG	ARG	614	42.274	14.328	48.621	1.00	58.30
	699	CD	ARG	614	42.908	14.348	47.242	1.00	60.57
15	700	NE	ARG	614	44.369	14.448	47.262	1.00	61.63
	701	CZ	ARG	614	45.056	15.421	47.868	1.00	63.66
	702	NH1	ARG	614	44.414	16.386	48.521	1.00	61.59
20	703	NH2	ARG	614	46.389	15.451	47.797	1.00	64.70
	704	C	ARG	614	39.440	16.960	48.776	1.00	58.09
	705	O	ARG	614	39.613	17.922	48.041	1.00	63.07
25	706	N	GLN	615	38.239	16.538	49.137	1.00	64.09
	707	CA	GLN	615	37.033	17.192	48.660	1.00	61.67
	708	CB	GLN	615	35.840	16.259	48.801	1.00	62.84
30	709	CG	GLN	615	35.738	15.162	47.795	1.00	62.14
	710	CD	GLN	615	34.290	14.775	47.573	1.00	58.76
	711	OE1	GLN	615	33.532	14.598	48.525	1.00	62.70
35	712	NE2	GLN	615	33.897	14.651	46.314	1.00	61.03
	713	C	GLN	615	36.677	18.478	49.396	1.00	59.82
	714	O	GLN	615	36.200	19.441	48.784	1.00	60.64
40	715	N	SER	616	36.901	18.480	50.709	1.00	62.12
	716	CA	SER	616	36.522	19.615	51.545	1.00	62.52
	717	CB	SER	616	35.199	19.297	52.239	1.00	61.86
45	718	OG	SER	616	35.408	18.310	53.240	1.00	59.96
	719	C	SER	616	37.514	20.090	52.612	1.00	61.77
	720	O	SER	616	37.110	20.501	53.703	1.00	63.13
50	721	N	SER	617	38.804	20.026	52.321	1.00	59.65
	722	CA	SER	617	39.796	20.502	53.279	1.00	60.19
	723	CB	SER	617	39.818	22.033	53.253	1.00	60.71
55	724	OG	SER	617	39.578	22.511	51.942	1.00	63.01
	725	C	SER	617	39.569	20.029	54.724	1.00	59.81
	726	O	SER	617	40.164	20.577	55.654	1.00	63.66
55	727	N	ALA	618	38.700	19.036	54.903	1.00	64.87
	728	CA	ALA	618	38.393	18.444	56.210	1.00	62.57
	729	CB	ALA	618	39.673	18.327	57.064	1.00	60.83
	730	C	ALA	618	37.277	19.059	57.053	1.00	59.66

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
731	O	ALA	618	37.238	18.817	58.260	1.00	60.80
732	N	ASN	619	36.375	19.839	56.451	1.00	63.98
733	CA	ASN	619	35.262	20.411	57.227	1.00	61.08
734	CB	ASN	619	35.129	21.934	57.042	1.00	61.69
735	CG	ASN	619	35.946	22.453	55.912	1.00	62.23
736	OD1	ASN	619	35.664	22.172	54.751	1.00	61.72
737	ND2	ASN	619	36.980	23.217	56.239	1.00	61.09
738	C	ASN	619	33.907	19.755	56.958	1.00	60.70
739	O	ASN	619	32.856	20.374	57.157	1.00	60.32
740	N	LEU	620	33.951	18.505	56.500	1.00	59.87
741	CA	LEU	620	32.767	17.686	56.237	1.00	59.97
742	CB	LEU	620	31.777	18.358	55.270	1.00	59.52
743	CG	LEU	620	32.162	19.088	53.990	1.00	61.28
744	CD1	LEU	620	31.041	18.989	52.971	1.00	64.28
745	CD2	LEU	620	32.459	20.539	54.330	1.00	65.45
746	C	LEU	620	33.147	16.307	55.712	1.00	61.40
747	O	LEU	620	33.869	16.178	54.720	1.00	61.10
748	N	LEU	621	32.660	15.280	56.407	1.00	58.95
749	CA	LEU	621	32.926	13.891	56.050	1.00	61.88
750	CB	LEU	621	32.394	12.947	57.123	1.00	63.38
751	CG	LEU	621	33.031	13.049	58.503	1.00	60.66
752	CD1	LEU	621	32.383	12.036	59.434	1.00	59.80
753	CD2	LEU	621	34.524	12.808	58.390	1.00	62.77
754	C	LEU	621	32.283	13.540	54.728	1.00	62.48
755	O	LEU	621	31.092	13.751	54.531	1.00	61.33
756	N	CYS	622	33.077	12.972	53.833	1.00	59.02
757	CA	CYS	622	32.585	12.609	52.523	1.00	62.42
758	CB	CYS	622	33.453	13.304	51.479	1.00	59.42
759	SG	CYS	622	33.715	15.064	51.889	1.00	59.94
760	C	CYS	622	32.566	11.094	52.329	1.00	59.63
761	O	CYS	622	33.248	10.552	51.451	1.00	58.28
762	N	PHE	623	31.766	10.421	53.156	1.00	62.39
763	CA	PHE	623	31.645	8.972	53.088	1.00	60.88
764	CB	PHE	623	-30.387	8.490	53.841	1.00	59.68
765	CG	PHE	623	30.461	8.686	55.344	1.00	58.52
766	CD1	PHE	623	30.338	9.948	55.906	1.00	66.23
767	CD2	PHE	623	30.688	7.612	56.191	1.00	63.42

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	768	CE1	PHE	623	30.443	10.139	57.292	1.00	60.25
	769	CE2	PHE	623	30.795	7.796	57.576	1.00	58.96
	770	CZ	PHE	623	30.673	9.059	58.124	1.00	57.60
10	771	C	PHE	623	31.618	8.532	51.630	1.00	61.75
	772	O	PHE	623	32.502	7.802	51.179	1.00	60.41
	773	N	ALA	624	30.624	8.995	50.888	1.00	64.49
15	774	CA	ALA	624	30.517	8.644	49.476	1.00	61.68
	775	CB	ALA	624	29.429	7.592	49.276	1.00	60.07
	776	C	ALA	624	30.179	9.912	48.700	1.00	60.93
20	777	O	ALA	624	30.002	10.981	49.297	1.00	60.98
	778	N	PRO	625	30.130	9.828	47.355	1.00	62.43
	779	CD	PRO	625	30.706	8.811	46.459	1.00	62.52
25	780	CA	PRO	625	29.795	11.035	46.593	1.00	59.45
	781	CB	PRO	625	29.949	10.582	45.146	1.00	62.18
	782	CG	PRO	625	31.089	9.653	45.245	1.00	59.91
30	783	C	PRO	625	28.366	11.397	46.928	1.00	62.94
	784	O	PRO	625	28.111	12.382	47.622	1.00	59.36
	785	N	ASP	626	27.433	10.572	46.468	1.00	58.86
35	786	CA	ASP	626	26.036	10.848	46.741	1.00	60.61
	787	CB	ASP	626	25.126	9.882	45.939	1.00	65.12
	788	CG	ASP	626	25.227	8.421	46.393	1.00	60.28
40	789	OD1	ASP	626	25.311	8.160	47.612	1.00	60.31
	790	OD2	ASP	626	25.189	7.526	45.518	1.00	59.51
	791	C	ASP	626	25.680	10.825	48.248	1.00	58.60
45	792	O	ASP	626	24.510	10.636	48.616	1.00	62.03
	793	N	LEU	627	26.668	11.051	49.119	1.00	63.43
	794	CA	LEU	627	26.392	11.020	50.552	1.00	61.63
50	795	CB	LEU	627	26.175	9.573	51.007	1.00	58.45
	796	CG	LEU	627	25.874	9.407	52.496	1.00	63.46
	797	CD1	LEU	627	24.401	9.669	52.770	1.00	60.41
55	798	CD2	LEU	627	26.241	8.013	52.919	1.00	65.05
	799	C	LEU	627	27.435	11.665	51.459	1.00	61.00
	800	O	LEU	627	28.320	10.988	51.985	1.00	62.27
	801	N	ILE	628	27.301	12.965	51.682	1.00	59.87
	802	CA	ILE	628	28.230	13.686	52.537	1.00	61.72
	803	CB	ILE	628	28.796	14.887	51.787	1.00	61.79
	804	CG2	ILE	628	29.848	15.575	52.618	1.00	61.82

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	805	CG1	ILE	628	29.391	14.418	50.461	1.00	58.81
	806	CD1	ILE	628	29.806	15.542	49.554	1.00	61.23
	807	C	ILE	628	27.541	14.162	53.815	1.00	59.57
	808	O	ILE	628	26.396	14.611	53.779	1.00	61.09
10	809	N	ILE	629	28.221	14.044	54.951	1.00	60.22
	810	CA	ILE	629	27.638	14.493	56.208	1.00	60.98
	811	CB	ILE	629	28.261	13.766	57.423	1.00	65.92
15	812	CG2	ILE	629	28.292	14.681	58.647	1.00	62.88
	813	CG1	ILE	629	27.419	12.536	57.768	1.00	64.60
	814	CD1	ILE	629	26.917	11.766	56.571	1.00	63.67
	815	C	ILE	629	27.852	15.989	56.319	1.00	60.46
20	816	O	ILE	629	28.935	16.452	56.676	1.00	60.38
	817	N	ASN	630	26.797	16.729	55.994	1.00	61.49
	818	CA	ASN	630	26.789	18.187	56.015	1.00	61.95
25	819	CB	ASN	630	25.655	18.685	55.149	1.00	60.74
	820	CG	ASN	630	24.348	18.042	55.516	1.00	63.39
	821	OD1	ASN	630	24.011	17.949	56.688	1.00	62.29
30	822	ND2	ASN	630	23.603	17.591	54.525	1.00	63.08
	823	C	ASN	630	26.616	18.786	57.402	1.00	63.46
	824	O	ASN	630	26.311	18.085	58.369	1.00	63.49
	825	N	GLU	631	26.794	20.103	57.475	1.00	60.97
35	826	CA	GLU	631	26.658	20.840	58.729	1.00	59.85
	827	CB	GLU	631	26.743	22.349	58.484	1.00	62.90
	828	CG	GLU	631	26.784	23.166	59.774	1.00	60.34
40	829	CD	GLU	631	25.819	24.340	59.761	1.00	60.36
	830	OE1	GLU	631	24.688	24.184	60.288	1.00	62.28
	831	OE2	GLU	631	26.191	25.406	59.213	1.00	56.78
	832	C	GLU	631	25.313	20.519	59.367	1.00	59.95
45	833	O	GLU	631	25.223	20.250	60.564	1.00	61.19
	834	N	GLN	632	24.268	20.540	58.552	1.00	60.53
	835	CA	GLN	632	22.933	20.248	59.046	1.00	60.62
50	836	CB	GLN	632	21.930	20.354	57.895	1.00	64.85
	837	CG	GLN	632	22.121	21.610	57.031	1.00	59.39
	838	CD	GLN	632	22.081	22.917	57.841	1.00	63.65
	839	OE1	GLN	632	21.068	23.248	58.473	1.00	59.92
55	840	NE2	GLN	632	23.193	23.663	57.821	1.00	62.67
	841	C	GLN	632	22.873	18.860	59.697	1.00	63.23

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	842	O	GLN	632	22.554	18.741	60.882	1.00	61.37
	843	N	ARG	633	23.213	17.827	58.929	1.00	62.09
	844	CA	ARG	633	23.190	16.444	59.406	1.00	61.43
10	845	CB	ARG	633	23.762	15.504	58.345	1.00	60.38
	846	CG	ARG	633	22.863	15.388	57.142	1.00	58.68
	847	CD	ARG	633	23.419	14.459	56.102	1.00	63.71
15	848	NE	ARG	633	22.589	14.486	54.905	1.00	62.14
	849	CZ	ARG	633	22.885	13.852	53.780	1.00	60.28
	850	NH1	ARG	633	23.996	13.136	53.704	1.00	60.27
20	851	NH2	ARG	633	22.075	13.937	52.733	1.00	60.98
	852	C	ARG	633	23.833	16.137	60.753	1.00	64.07
	853	O	ARG	633	23.495	15.117	61.348	1.00	60.29
25	854	N	MET	634	24.758	16.970	61.236	1.00	61.53
	855	CA	MET	634	25.334	16.721	62.560	1.00	60.63
	856	CB	MET	634	26.429	17.747	62.859	1.00	60.06
30	857	CG	MET	634	27.598	17.688	61.874	1.00	53.30
	858	SD	MET	634	28.604	16.178	62.057	1.00	63.04
	859	CE	MET	634	30.133	16.562	61.162	1.00	60.95
35	860	C	MET	634	24.150	16.834	63.555	1.00	60.65
	861	O	MET	634	23.899	17.897	64.149	1.00	63.14
	862	N	THR	635	23.420	15.714	63.670	1.00	63.54
40	863	CA	THR	635	22.220	15.523	64.504	1.00	61.73
	864	CB	THR	635	21.180	14.557	63.819	1.00	59.70
	865	OG1	THR	635	20.987	14.911	62.442	1.00	57.94
45	866	CG2	THR	635	19.829	14.609	64.552	1.00	63.34
	867	C	THR	635	22.593	14.861	65.825	1.00	61.33
	868	O	THR	635	23.570	15.251	66.464	1.00	63.49
50	869	N	LEU	636	21.796	13.851	66.198	1.00	60.18
	870	CA	LEU	636	21.953	13.057	67.420	1.00	61.62
	871	CB	LEU	636	22.112	11.577	67.095	1.00	60.70
55	872	CG	LEU	636	22.867	10.855	68.213	1.00	62.64
	873	CD1	LEU	636	21.904	10.048	69.070	1.00	63.15
	874	CD2	LEU	636	23.910	9.960	67.603	1.00	60.79
55	875	C	LEU	636	23.183	13.478	68.172	1.00	61.59
	876	O	LEU	636	24.287	13.372	67.626	1.00	60.57
	877	N	PRO	637	23.029	13.907	69.442	1.00	59.83
	878	CD	PRO	637	22.008	13.402	70.379	1.00	57.71

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
879	CA	PRO	637	24.225	14.321	70.182	1.00	61.11
880	CB	PRO	637	23.810	14.133	71.639	1.00	61.28
881	CG	PRO	637	22.862	12.966	71.555	1.00	61.68
882	C	PRO	637	25.417	13.433	69.793	1.00	61.18
883	O	PRO	637	26.457	13.928	69.331	1.00	61.45
884	N	CYS	638	25.243	12.117	69.920	1.00	63.53
885	CA	CYS	638	26.333	11.211	69.588	1.00	61.78
886	CB	CYS	638	26.024	9.787	70.065	1.00	62.20
887	SG	CYS	638	24.449	9.498	70.917	1.00	60.82
888	C	CYS	638	26.722	11.209	68.101	1.00	61.50
889	O	CYS	638	27.863	10.844	67.765	1.00	61.11
890	N	MET	639	25.816	11.625	67.214	1.00	57.65
891	CA	MET	639	26.186	11.638	65.817	1.00	60.56
892	CB	MET	639	25.103	12.211 1	64.924	1.00	66.32
893	CG	MET	639	25.612	12.161	63.532	1.00	60.47
894	SD	MET	639	25.084	11.084	62.238	1.00	57.31
895	CE	MET	639	25.984	11.962	61.115	1.00	58.45
896	C	MET	639	27.478	12.449	65.637	1.00	62.26
897	O	MET	639	28.361	12.083	64.857	1.00	61.35
898	N	TYR	640	27.589	13.543	66.383	1.00	61.78
899	CA	TYR	640	28.797	14.339	66.340	1.00	61.48
900	CB	TYR	640	28.569	15.755	66.872	1.00	60.05
901	CG	TYR	640	29.871	16.511	66.956	1.00	61.42
902	CD1	TYR	640	30.530	16.927	65.795	1.00	62.42
903	CE1	TYR	640	31.800	17.472	65.846	1.00	61.93
904	CD2	TYR	640	30.519	16.680	68.175	1.00	59.45
905	CE2	TYR	640	31.785	17.222	68.235	1.00	63.13
906	CZ	TYR	640	32.425	17.612	67.068	1.00	58.88
907	OH	TYR	640	33.711	18.103	67.130	1.00	60.76
908	C	TYR	640	29.842	13.646	67.215	1.00	60.30
909	O	TYR	640	31.041	13.847	67.034	1.00	63.06
910	N	ASP	641	29.397	12.830	68.168	1.00	61.14
911	CA	ASP	641	30.349	12.136	69.035	1.00	62.18
912	CB	ASP	641	29.674	11.669	70.323	1.00	59.68
913	CG	ASP	641	29.145	12.828	71.135	1.00	60.96
914	OD1	ASP	641	27.930	13.090	71.062	1.00	61.07
915	OD2	ASP	641	29.950	13.493	71.824	1.00	63.74

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	916	C	ASP	641	30.991	10.971	68.313	1.00	60.81
	917	O	ASP	641	32.047	10.482	68.721	1.00	60.52
	918	N	GLN	642	30.349	10.542	67.229	1.00	59.76
10	919	CA	GLN	642	30.860	9.456	66.396	1.00	63.97
	920	CB	GLN	642	29.721	8.763	65.687	1.00	61.51
	921	CG	GLN	642	28.690	8.348	66.642	1.00	61.79
15	922	CD	GLN	642	27.547	7.724	65.978	1.00	62.69
	923	OE1	GLN	642	27.709	6.684	65.308	1.00	61.01
	924	NE2	GLN	642	26.355	8.326	66.145	1.00	60.03
20	925	C	GLN	642	31.766	10.069	65.359	1.00	62.81
	926	O	GLN	642	32.954	9.760	65.294	1.00	61.10
	927	N	CYS	643	31.190	10.957	64.556	1.00	60.88
25	928	CA	CYS	643	31.931	11.628	63.504	1.00	61.65
	929	CB	CYS	643	30.977	12.508	62.694	1.00	61.95
	930	SG	CYS	643	29.662	11.585	61.843	1.00	63.26
30	931	C	CYS	643	33.081	12.455	64.071	1.00	61.30
	932	O	CYS	643	34.102	12.652	63.418	1.00	61.90
	933	N	LYS	644	32.911	12.923	65.299	1.00	62.82
35	934	CA	LYS	644	33.923	13.730	65.951	1.00	58.73
	935	CB	LYS	644	33.634	13.827	67.449	1.00	63.83
	936	CG	LYS	644	34.630	14.686	68.207	1.00	59.96
40	937	CD	LYS	644	34.226	14.891	69.665	1.00	59.57
	938	CE	LYS	644	35.160	15.902	70.358	1.00	59.22
	939	NZ	LYS	644	35.201	17.239	69.668	1.00	61.66
45	940	C	LYS	644	35.328	13.182	65.747	1.00	61.72
	941	O	LYS	644	36.296	13.941	65.673	1.00	61.77
	942	N	HIS	645	35.451	11.864	65.655	1.00	61.41
50	943	CA	HIS	645	36.769	11.262	65.474	1.00	59.96
	944	CB	HIS	645	36.856	9.943	66.209	1.00	60.26
	945	CG	HIS	645	37.109	10.100	67.667	1.00	59.75
55	946	CD2	HIS	645	38.254	10.338	68.346	1.00	58.42
	947	ND1	HIS	645	36.103	10.041	68.606	1.00	61.77
	948	CE1	HIS	645	36.621	10.232	69.805	1.00	58.75
55	949	NE2	HIS	645	37.924	10.415	69.675	1.00	57.48
	950	C	HIS	645	37.165	11.038	64.037	1.00	60.84
	951	O	HIS	645	38.352	11.000	63.727	1.00	62.12
	952	N	MET	646	36.172	10.856	63.174	1.00	63.11

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	953	CA	MET	646	36.432	10.651	61.759	1.00	62.74
	954	CB	MET	646	35.135	10.211	61.023	1.00	61.50
	955	CG	MET	646	34.686	8.771	61.338	1.00	58.88
	956	SD	MET	646	32.994	8.315	60.876	1.00	61.92
10	957	CE	MET	646	32.426	8.134	62.441	1.00	62.24
	958	C	MET	646	36.948	11.972	61.168	1.00	63.61
	959	O	MET	646	37.709	11.962	60.197	1.00	63.12
15	960	N	LEU	647	36.543	13.093	61.772	1.00	60.39
	961	CA	LEU	647	36.963	14.419	61.325	1.00	61.16
	962	CB	LEU	647	36.105	15.510	61.965	1.00	62.09
	963	CG	LEU	647	34.661	15.778	61.551	1.00	62.69
20	964	CD1	LEU	647	34.144	16.850	62.479	1.00	59.66
	965	CD2	LEU	647	34.553	16.232	60.098	1.00	61.60
	966	C	LEU	647	38.400	14.652	61.731	1.00	62.99
25	967	O	LEU	647	39.164	15.329	61.042	1.00	62.41
	968	N	TYR	648	38.750	14.087	62.876	1.00	60.24
	969	CA	TYR	648	40.087	14.202	63.431	1.00	60.92
30	970	CB	TYR	648	40.190	13.339	64.685	1.00	59.63
	971	CG	TYR	648	41.486	13.510	65.428	1.00	60.33
	972	CD1	TYR	648	42.672	12.950	64.952	1.00	62.96
	973	CE1	TYR	648	43.876	13.160	65.609	1.00	61.51
35	974	CD2	TYR	648	41.537	14.280	66.585	1.00	57.67
	975	CE2	TYR	648	42.735	14.500	67.252	1.00	62.62
	976	CZ	TYR	648	43.902	13.938	66.759	1.00	60.16
40	977	OH	TYR	648	45.089	14.157	67.426	1.00	64.40
	978	C	TYR	648	41.164	13.787	62.435	1.00	61.32
	979	O	TYR	648	42.045	14.575	62.099	1.00	62.83
45	980	N	VAL	649	41.107	12.545	61.971	1.00	65.90
	981	CA	VAL	649	42.105	12.079	61.027	1.00	60.14
	982	CB	VAL	649	41.862	10.578	60.642	1.00	59.02
	983	CG1	VAL	649	40.528	10.109	61.218	1.00	60.92
50	984	CG2	VAL	649	41.930	10.372	59.122	1.00	59.70
	985	C	VAL	649	42.072	12.982	59.814	1.00	61.99
	986	O	VAL	649	43.105	13.378	59.297	1.00	60.55
55	987	N	SER	650	40.873	13.339	59.390	1.00	61.60
	988	CA	SER	650	40.705	14.191	58.226	1.00	61.66
	989	CB	SER	650	39.224	14.356	57.914	1.00	61.34

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	990	OG	SER	650	39.069	14.979	56.662	1.00	64.56
	991	C	SER	650	41.344	15.555	58.429	1.00	61.44
	992	O	SER	650	41.800	16.181	57.476	1.00	58.88
10	993	N	SER	651	41.365	16.013	59.677	1.00	59.26
	994	CA	SER	651	41.960	17.298	60.029	1.00	62.47
	995	CB	SER	651	41.578	17.637	61.483	1.00	58.62
15	996	OG	SER	651	42.537	18.441	62.154	1.00	60.41
	997	C	SER	651	43.480	17.204	59.849	1.00	61.76
	998	O	SER	651	44.087	18.019	59.164	1.00	62.09
20	999	N	GLU	652	44.070	16.172	60.441	1.00	60.41
	1000	CA	GLU	652	45.509	15.927	60.395	1.00	60.48
	1001	CB	GLU	652	45.837	14.680	61.220	1.00	65.10
25	1002	CG	GLU	652	45.488	14.822	62.677	1.00	59.36
	1003	CD	GLU	652	46.160	16.021	63.289	1.00	62.29
	1004	OE1	GLU	652	47.399	15.970	63.444	1.00	60.10
30	1005	OE2	GLU	652	45.451	17.014	63.592	1.00	60.61
	1006	C	GLU	652	46.100	15.773	59.001	1.00	59.16
	1007	O	GLU	652	47.238	16.166	58.755	1.00	59.92
35	1008	N	LEU	653	45.335	15.180	58.094	1.00	60.01
	1009	CA	LEU	653	45.807	14.984	56.731	1.00	61.61
	1010	CB	LEU	653	44.874	14.048	55.960	1.00	64.78
40	1011	CG	LEU	653	44.860	12.600	56.432	1.00	63.03
	1012	CD1	LEU	653	43.723	11.868	55.768	1.00	60.96
	1013	CD2	LEU	653	46.179	11.941	56.122	1.00	62.70
45	1014	C	LEU	653	45.878	16.328	56.037	1.00	60.72
	1015	O	LEU	653	46.805	16.588	55.269	1.00	61.12
	1016	N	HIS	654	44.895	17.182	56.303	1.00	62.78
50	1017	CA	HIS	654	44.894	18.497	55.698	1.00	61.32
	1018	CB	HIS	654	43.513	19.141	55.805	1.00	63.28
	1019	CG	HIS	654	43.517	20.607	55.518	1.00	61.88
55	1020	CD2	HIS	654	43.210	21.296	54.394	1.00	59.76
	1021	ND1	HIS	654	43.946	21.543	56.436	1.00	58.15
	1022	CE1	HIS	654	43.905	22.744	55.889	1.00	62.74
60	1023	NE2	HIS	654	43.463	22.622	54.650	1.00	60.79
	1024	C	HIS	654	45.935	19.319	56.440	1.00	62.39
	1025	O	HIS	654	46.667	20.112	55.851	1.00	62.10
65	1026	N	ARG	655	46.012	19.098	57.743	1.00	62.07

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	1027	CA	ARG	655	46.968	19.804	58.572	1.00	62.85
	1028	CB	ARG	655	46.882	19.277	60.008	1.00	58.45
	1029	CG	ARG	655	47.082	20.314	61.111	1.00	57.53
10	1030	CD	ARG	655	48.522	20.368	61.565	1.00	58.48
	1031	NE	ARG	655	48.968	19.079	62.082	1.00	61.43
	1032	CZ	ARG	655	50.206	18.831	62.503	1.00	59.99
15	1033	NH1	ARG	655	51.125	19.790	62.472	1.00	61.84
	1034	NH2	ARG	655	50.537	17.625	62.950	1.00	60.75
	1035	C	ARG	655	48.367	19.599	57.999	1.00	60.66
20	1036	O	ARG	655	49.086	20.566	57.753	1.00	62.69
	1037	N	LEU	656	48.735	18.340	57.759	1.00	60.05
	1038	CA	LEU	656	50.060	18.008	57.224	1.00	61.69
25	1039	CB	LEU	656	50.575	16.697	57.832	1.00	60.63
	1040	CG	LEU	656	50.902	16.651	59.330	1.00	60.12
	1041	CD1	LEU	656	51.059	15.205	59.759	1.00	61.83
30	1042	CD2	LEU	656	52.161	17.440	59.632	1.00	61.33
	1043	C	LEU	656	50.164	17.922	55.706	1.00	60.82
	1044	O	LEU	656	51.187	17.491	55.184	1.00	63.77
35	1045	N	GLN	657	49.119	18.321	54.995	1.00	62.25
	1046	CA	GLN	657	49.165	18.291	53.543	1.00	62.13
	1047	CB	GLN	657	50.018	19.442	53.026	1.00	59.95
40	1048	CG	GLN	657	49.412	20.805	53.219	1.00	60.54
	1049	CD	GLN	657	48.109	20.944	52.480	1.00	59.94
	1050	OE1	GLN	657	47.043	20.616	52.997	1.00	61.59
45	1051	NE2	GLN	657	48.189	21.413	51.250	1.00	59.69
	1052	C	GLN	657	49.756	16.998	53.027	1.00	64.37
	1053	O	GLN	657	50.684	17.013	52.230	1.00	60.80
50	1054	N	VAL	658	49.233	15.876	53.487	1.00	59.26
	1055	CA	VAL	658	49.730	14.589	53.048	1.00	60.79
	1056	CB	VAL	658	49.044	13.466	53.856	1.00	61.35
55	1057	CG1	VAL	658	49.169	12.130	53.154	1.00	61.79
	1058	CG2	VAL	658	49.663	13.406	55.240	1.00	61.37
	1059	C	VAL	658	49.494	14.416	51.552	1.00	60.15
55	1060	O	VAL	658	48.452	14.798	51.025	1.00	60.95
	1061	N	SER	659	50.485	13.862	50.869	1.00	63.41
	1062	CA	SER	659	50.399	13.615	49.438	1.00	58.10
	1063	CB	SER	659	51.797	13.685	48.834	1.00	59.86

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1064	OG	SER	659	52.018	12.643	47.905	1.00	62.03
	1065	C	SER	659	49.777	12.242	49.157	1.00	62.11
	1066	O	SER	659	49.781	11.353	50.015	1.00	61.38
10	1067	N	TYR	660	49.243	12.062	47.956	1.00	60.30
	1068	CA	TYR	660	48.633	10.789	47.601	1.00	61.68
	1069	CB	TYR	660	48.100	10.860	46.177	1.00	61.85
15	1070	CG	TYR	660	47.411	9.605	45.727	1.00	59.67
	1071	CD1	TYR	660	46.561	8.911	46.581	1.00	63.51
	1072	CE1	TYR	660	45.893	7.783	46.152	1.00	60.60
20	1073	CD2	TYR	660	47.576	9.134	44.431	1.00	60.37
	1074	CE2	TYR	660	46.911	8.011	43.990	1.00	64.13
	1075	CZ	TYR	660	46.072	7.339	44.851	1.00	63.85
25	1076	OH	TYR	660	45.393	6.229	44.402	1.00	62.07
	1077	C	TYR	660	49.584	9.594	47.749	1.00	59.81
	1078	O	TYR	660	49.175	8.510	48.165	1.00	64.86
30	1079	N	GLU	661	50.853	9.789	47.411	1.00	60.25
	1080	CA	GLU	661	51.814	8.703	47.527	1.00	62.48
	1081	CB	GLU	661	53.119	9.034	46.788	1.00	61.23
35	1082	CG	GLU	661	53.209	8.405	45.395	1.00	63.67
	1083	CD	GLU	661	54.517	8.708	44.672	1.00	65.78
	1084	OE1	GLU	661	55.602	8.472	45.247	1.00	60.21
40	1085	OE2	GLU	661	54.462	9.174	43.517	1.00	60.28
	1086	C	GLU	661	52.096	8.354	48.980	1.00	61.69
	1087	O	GLU	661	52.247	7.183	49.312	1.00	61.32
45	1088	N	GLU	662	52.160	9.348	49.854	1.00	62.68
	1089	CA	GLU	662	52.405	9.048	51.252	1.00	63.61
	1090	CB	GLU	662	52.605	10.340	52.032	1.00	61.04
50	1091	CG	GLU	662	53.485	11.321	51.309	1.00	61.12
	1092	CD	GLU	662	53.768	12.555	52.117	1.00	62.85
	1093	OE1	GLU	662	52.822	13.164	52.637	1.00	58.86
55	1094	OE2	GLU	662	54.945	12.931	52.227	1.00	61.02
	1095	C	GLU	662	51.193	8.277	51.784	1.00	59.86
	1096	O	GLU	662	51.333	7.263	52.466	1.00	63.08
60	1097	N	TYR	663	50.007	8.771	51.436	1.00	61.62
	1098	CA	TYR	663	48.716	8.186	51.812	1.00	62.54
	1099	CB	TYR	663	47.601	8.921	51.068	1.00	63.89
65	1100	CG	TYR	663	46.266	8.230	51.167	1.00	61.84

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1101	CD1	TYR	663	45.619	8.109	52.392	1.00	59.60
1102	CE1	TYR	663	44.407	7.458	52.498	1.00	58.52
1103	CD2	TYR	663	45.659	7.676	50.043	1.00	58.65
1104	CE2	TYR	663	44.441	7.019	50.138	1.00	60.83
1105	CZ	TYR	663	43.820	6.916	51.368	1.00	62.58
1106	OH	TYR	663	42.601	6.287	51.477	1.00	61.21
1107	C	TYR	663	48.565	6.680	51.537	1.00	59.94
1108	O	TYR	663	48.090	5.918	52.389	1.00	60.92
1109	N	LEU	664	48.930	6.274	50.325	1.00	60.84
1110	CA	LEU	664	48.846	4.881	49.908	1.00	61.56
1111	CB	LEU	664	49.261	4.757	48.438	1.00	60.37
1112	CG	LEU	664	48.363	5.402	47.382	1.00	64.33
1113	CD1	LEU	664	49.036	5.350	46.023	1.00	64.49
1114	CD2	LEU	664	47.032	4.687	47.351	1.00	59.02
1115	C	LEU	664	49.744	4.001	50.777	1.00	60.21
1116	O	LEU	664	49.369	2.889	51.161	1.00	61.89
1117	N	CYS	665	50.933	4.519	51.071	1.00	61.72
1118	CA	CYS	665	51.915	3.823	51.882	1.00	58.12
1119	CB	CYS	665	53.272	4.508	51.737	1.00	62.31
1120	SG	CYS	665	54.006	4.295	50.123	1.00	59.12
1121	C	CYS	665	51.516	3.771	53.348	1.00	59.84
1122	O	CYS	665	51.726	2.766	54.024	1.00	61.71
1123	N	MET	666	50.953	4.862	53.845	1.00	63.34
1124	CA	MET	666	50.524	4.910	55.228	1.00	58.59
1125	CB	MET	666	50.199	6.341	55.627	1.00	59.71
1126	CG	MET	666	51.408	7.189	55.867	1.00	62.55
1127	SD	MET	666	50.921	8.891	56.036	1.00	61.95
1128	CE	MET	666	50.313	8.927	57.659	1.00	64.15
1129	C	MET	666	49.303	4.023	55.437	1.00	63.86
1130	O	MET	666	49.146	3.420	56.495	1.00	59.48
1131	N	LYS	667	48.446	3.950	54.421	1.00	58.08
1132	CA	LYS	667	47.241	3.129	54.482	1.00	61.17
1133	CB	LYS	667	46.318	3.429	53.305	1.00	66.33
1134	CG	LYS	667	45.013	2.663	53.338	1.00	59.73
1135	CD	LYS	667	43.951	3.382	52.532	1.00	60.07
1136	CE	LYS	667	44.313	3.462	51.063	1.00	62.82
1137	NZ	LYS	667	44.134	2.158	50.390	1.00	62.44

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1138	C	LYS	667	47.592	1.658	54.468	1.00	63.84
	1139	O	LYS	667	46.867	0.838	55.011	1.00	61.95
	1140	N	THR	668	48.705	1.318	53.838	1.00	63.32
10	1141	CA	THR	668	49.114	-0.069	53.801	1.00	61.88
	1142	CB	THR	668	50.080	-0.304	52.657	1.00	60.27
	1143	OG1	THR	668	49.463	0.124	51.439	1.00	62.16
15	1144	CG2	THR	668	50.417	-1.775	52.547	1.00	58.76
	1145	C	THR	668	49.761	-0.413	55.137	1.00	62.68
	1146	O	THR	668	49.707	-1.559	55.591	1.00	62.61
20	1147	N	LEU	669	50.350	0.597	55.773	1.00	62.26
	1148	CA	LEU	669	50.995	0.427	57.068	1.00	61.58
	1149	CB	LEU	669	51.888	1.626	57.378	1.00	62.50
25	1150	CG	LEU	669	53.265	1.643	56.712	1.00	57.56
	1151	CD1	LEU	669	54.041	2.847	57.205	1.00	60.97
	1152	CD2	LEU	669	54.012	0.355	57.037	1.00	59.22
30	1153	C	LEU	669	49.987	0.249	58.194	1.00	61.00
	1154	O	LEU	669	50.354	-0.119	59.310	1.00	61.30
	1155	N	LEU	670	48.718	0.520	57.911	1.00	62.31
35	1156	CA	LEU	670	47.686	0.365	58.925	1.00	62.17
	1157	CB	LEU	670	46.511	1.305	58.638	1.00	64.37
	1158	CG	LEU	670	46.784	2.784	58.942	1.00	60.87
40	1159	CD1	LEU	670	45.516	3.597	58.766	1.00	63.22
	1160	CD2	LEU	670	47.293	2.922	60.365	1.00	58.85
	1161	C	LEU	670	47.227	-1.090	58.976	1.00	63.40
45	1162	O	LEU	670	46.846	-1.599	60.026	1.00	63.58
	1163	N	LEU	671	47.281	-1.750	57.827	1.00	61.89
	1164	CA	LEU	671	46.913	-3.150	57.716	1.00	60.74
50	1165	CB	LEU	671	46.946	-3.574	56.249	1.00	62.54
	1166	CG	LEU	671	46.501	-4.997	55.921	1.00	62.48
	1167	CD1	LEU	671	45.015	-5.180	56.251	1.00	63.63
55	1168	CD2	LEU	671	46.768	-5.260	54.449	1.00	63.52
	1169	C	LEU	671	47.967	-3.928	58.500	1.00	61.46
	1170	O	LEU	671	47.688	-4.971	59.110	1.00	60.81
55	1171	N	LEU	672	49.182	-3.388	58.479	1.00	62.75
	1172	CA	LEU	672	50.320	-3.974	59.163	1.00	62.92
	1173	CB	LEU	672	51.562	-3.883	58.280	1.00	60.56
	1174	CG	LEU	672	51.399	-4.164	56.786	1.00	62.90

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1175	CD1	LEU	672	52.776	-4.394	56.183	1.00	60.90
1176	CD2	LEU	672	50.519	-5.373	56.558	1.00	61.77
1177	C	LEU	672	50.576	-3.232	60.468	1.00	61.14
1178	O	LEU	672	51.722	-3.064	60.883	1.00	63.28
1179	N	SER	673	49.502	-2.795	61.116	1.00	62.86
1180	CA	SER	673	49.616	-2.056	62.368	1.00	62.27
1181	CB	SER	673	48.582	-0.910	62.405	1.00	61.42
1182	OG	SER	673	47.241	-1.383	62.404	1.00	59.49
1183	C	SER	673	49.468	-2.925	63.616	1.00	63.23
1184	O	SER	673	50.026	-2.608	64.664	1.00	59.71
1185	N	SER	674	48.720	-4.017	63.517	1.00	61.92
1186	CA	SER	674	48.538	-4.875	64.680	1.00	60.38
1187	CB	SER	674	47.225	-4.506	65.401	1.00	62.70
1188	OG	SER	674	46.204	-4.115	64.495	1.00	56.91
1189	C	SER	674	48.590	-6.373	64.405	1.00	61.52
1190	O	SER	674	48.122	-6.849	63.377	1.00	61.47
1191	N	VAL	675	49.192	-7.101	65.336	1.00	64.16
1192	CA	VAL	675	49.305	-8.556	65.256	1.00	61.09
1193	CB	VAL	675	50.722	-9.025	64.816	1.00	62.88
1194	CG1	VAL	675	50.962	-8.679	63.362	1.00	59.26
1195	CG2	VAL	675	51.787	-8.394	65.710	1.00	61.45
1196	C	VAL	675	49.039	-9.116	66.652	1.00	62.60
1197	O	VAL	675	49.265	-8.433	67.656	1.00	61.24
1198	N	PRO	676	48.550	-10.363	66.735	1.00	59.77
1199	CD	PRO	676	48.219	-11.265	65.616	1.00	57.51
1200	CA	PRO	676	48.260	-11.001	68.020	1.00	62.72
1201	CB	PRO	676	48.026	-12.452	67.623	1.00	60.61
1202	CG	PRO	676	47.362	-12.317	66.283	1.00	59.30
1203	C	PRO	676	49.424	-10.847	68.994	1.00	61.35
1204	O	PRO	676	50.585	-10.758	68.576	1.00	63.84
1205	N	LYS	677	49.117	-10.818	70.290	1.00	62.54
1206	CA	LYS	677	50.154	-10.673	71.314	1.00	60.54
1207	CB	LYS	677	49.510	-10.646	72.702	1.00	61.63
1208	CG	LYS	677	50.472	-10.433	73.853	1.00	58.65
1209	CD	LYS	677	49.861	-10.969	75.143	1.00	62.01
1210	CE	LYS	677	50.912	-11.109	76.241	1.00	63.79
1211	NZ	LYS	677	50.350	-11.727	77.491	1.00	60.49.

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1212	C	LYS	677	51.162	-11.828	71.222	1.00	61.45
	1213	O	LYS	677	52.102	-11.917	72.023	1.00	59.62
	1214	N	ASP	678	50.955	-12.698	70.231	1.00	59.93
10	1215	CA	ASP	678	51.809	-13.862	69.994	1.00	60.14
	1216	CB	ASP	678	51.041	-15.126	70.367	1.00	60.09
	1217	CG	ASP	678	50.390	-15.023	71.735	1.00	61.43
15	1218	OD1	ASP	678	51.110	-14.940	72.749	1.00	62.42
	1219	OD2	ASP	678	49.151	-15.016	71.797	1.00	60.77
	1220	C	ASP	678	52.273	-13.947	68.535	1.00	63.29
20	1221	O	ASP	678	52.771	-14.981	68.090	1.00	59.36
	1222	N	GLY	679	52.098	-12.854	67.797	1.00	59.82
	1223	CA	GLY	679	52.512	-12.823	66.408	1.00	58.14
25	1224	C	GLY	679	51.639	-13.640	65.481	1.00	58.50
	1225	O	GLY	679	50.600	-14.179	65.870	1.00	58.88
	1226	N	LEU	680	52.082	-13.723	64.237	1.00	62.95
30	1227	CA	LEU	680	51.375	-14.459	63.209	1.00	63.18
	1228	CB	LEU	680	51.233	-13.564	61.981	1.00	65.44
	1229	CG	LEU	680	50.941	-12.101	62.324	1.00	60.24
35	1230	CD1	LEU	680	50.994	-11.260	61.069	1.00	60.21
	1231	CD2	LEU	680	49.582	-11.979	62.974	1.00	60.11
	1232	C	LEU	680	52.221	-15.685	62.881	1.00	63.74
40	1233	O	LEU	680	53.430	-15.689	63.110	1.00	62.10
	1234	N	LYS	681	51.598	-16.729	62.354	1.00	60.36
	1235	CA	LYS	681	52.348	-17.922	62.000	1.00	60.78
45	1236	CB	LYS	681	51.406	-18.969	61.418	1.00	60.11
	1237	CG	LYS	681	50.209	-19.253	62.289	1.00	61.43
	1238	CD	LYS	681	49.295	-20.221	61.579	1.00	63.30
50	1239	CE	LYS	681	47.908	-20.186	62.160	1.00	61.77
	1240	NZ	LYS	681	46.983	-20.886	61.244	1.00	62.13
	1241	C	LYS	681	53.429	-17.551	60.973	1.00	61.58
55	1242	O	LYS	681	54.401	-18.286	60.784	1.00	63.01
	1243	N	SER	682	53.250	-16.410	60.309	1.00	60.35
	1244	CA	SER	682	54.211	-15.932	59.314	1.00	62.36
	1245	CB	SER	682	53.515	-15.613	57.989	1.00	61.24
	1246	OG	SER	682	53.066	-16.788	57.346	1.00	63.18
	1247	C	SER	682	54.885	-14.674	59.826	1.00	64.68
	1248	O	SER	682	55.289	-13.814	59.051	1.00	59.53

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1249	N	GLN	683	55.012	-14.579	61.140	1.00	64.92
1250	CA	GLN	683	55.614	-13.411	61.754	1.00	62.89
1251	CB	GLN	683	55.862	-13.679	63.240	1.00	63.65
1252	CG	GLN	683	56.282	-12.452	64.059	1.00	64.38
1253	CD	GLN	683	55.318	-11.274	63.954	1.00	64.26
1254	OE1	GLN	683	55.688	-10.205	63.476	1.00	63.72
1255	NE2	GLN	683	54.085	-11.465	64.407	1.00	61.52
1256	C	GLN	683	56.893	-12.938	61.069	1.00	60.69
1257	O	GLN	683	56.981	-11.782	60.669	1.00	62.35
1258	N	GLU	684	57.880	-13.811	60.913	1.00	60.59
1259	CA	GLU	684	59.119	-13.378	60.279	1.00	61.72
1260	CB	GLU	684	60.039	-14.567	59.970	1.00	61.83
1261	CG	GLU	684	60.015	-15.013	58.511	1.00	61.93
1262	CD	GLU	684	61.383	-15.418	57.979	1.00	60.75
1263	OE1	GLU	684	61.457	-15.813	56.792	1.00	60.52
1264	OE2	GLU	684	62.375	-15.342	58.744	1.00	58.72
1265	C	GLU	684	58.801	-12.623	58.993	1.00	60.55
1266	O	GLU	684	59.196	-11.474	58.823	1.00	63.55
1267	N	LEU	685	58.064	-13.263	58.100	1.00	63.64
1268	CA	LEU	685	57.710	-12.649	56.834	1.00	57.80
1269	CB	LEU	685	56.921	-13.649	55.985	1.00	59.68
1270	CG	LEU	685	57.165	-13.734	54.476	1.00	63.20
1271	CD1	LEU	685	55.839	-14.063	53.829	1.00	59.43
1272	CD2	LEU	685	57.699	-12.434	53.902	1.00	62.25
1273	C	LEU	685	56.882	-11.370	57.040	1.00	62.31
1274	O	LEU	685	56.953	-10.432	56.242	1.00	61.77
1275	N	PHE	686	56.095	-11.326	58.109	1.00	60.23
1276	CA	PHE	686	55.272	-10.149	58.374	1.00	61.37
1277	CB	PHE	686	54.409	-10.365	59.609	1.00	64.14
1278	CG	PHE	686	53.663	-9.143	60.023	1.00	61.62
1279	CD1	PHE	686	52.639	-8.650	59.236	1.00	60.24
1280	CD2	PHE	686	54.008	-8.460	61.178	1.00	62.13
1281	CE1	PHE	686	51.971	-7.493	59.592	1.00	58.68
1282	CE2	PHE	686	53.347	-7.304	61.543	1.00	61.95
1283	CZ	PHE	686	52.326	-6.818	60.749	1.00	61.43
1284	C	PHE	686	56.109	-8.897	58.596	1.00	59.14
1285	O	PHE	686	56.247	-8.051	57.714	1.00	61.44

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1286	N	ASP	687	56.651	-8.791	59.802	1.00	64.05
	1287	CA	ASP	687	57.483	-7.668	60.195	1.00	60.85
	1288	CB	ASP	687	58.102	-7.960	61.567	1.00	56.84
10	1289	CG	ASP	687	59.033	-9.162	61.536	1.00	64.67
	1290	OD1	ASP	687	59.482	-9.610	62.622	1.00	60.21
	1291	OD2	ASP	687	59.322	-9.655	60.414	1.00	63.02
15	1292	C	ASP	687	58.573	-7.383	59.142	1.00	61.59
	1293	O	ASP	687	59.262	-6.358	59.214	1.00	61.60
	1294	N	GLU	688	58.725	-8.289	58.172	1.00	60.82
20	1295	CA	GLU	688	59.700	-8.104	57.098	1.00	59.68
	1296	CB	GLU	688	60.246	-9.433	56.604	1.00	62.54
	1297	CG	GLU	688	61.434	-9.252	55.674	1.00	60.98
25	1298	CD	GLU	688	61.479	-10.289	54.569	1.00	58.58
	1299	OE1	GLU	688	61.323	-9.898	53.387	1.00	61.73
	1300	OE2	GLU	688	61.663	-11.490	54.882	1.00	60.24
30	1301	C	GLU	688	59.031	-7.387	55.931	1.00	60.97
	1302	O	GLU	688	59.684	-6.719	55.137	1.00	62.27
	1303	N	ILE	689	57.721	-7.552	55.809	1.00	61.23
35	1304	CA	ILE	689	56.979	-6.864	54.767	1.00	61.00
	1305	CB	ILE	689	55.641	-7.592	54.451	1.00	63.41
	1306	CG2	ILE	689	54.655	-6.650	53.759	1.00	59.25
40	1307	CG1	ILE	689	55.916	-8.808	53.568	1.00	57.54
	1308	CD1	ILE	689	54.667	-9.526	53.121	1.00	62.29
	1309	C	ILE	689	56.704	-5.479	55.345	1.00	58.97
45	1310	O	ILE	689	56.778	-4.473	54.645	1.00	61.54
	1311	N	ARG	690	56.411	-5.439	56.641	1.00	60.16
	1312	CA	ARG	690	56.135	-4.185	57.319	1.00	61.28
50	1313	CB	ARG	690	55.855	-4.434	58.799	1.00	60.29
	1314	CG	ARG	690	55.548	-3.170	59.582	1.00	60.74
	1315	CD	ARG	690	54.679	-3.480	60.770	1.00	56.91
55	1316	NE	ARG	690	54.190	-2.280	61.437	1.00	66.99
	1317	CZ	ARG	690	54.967	-1.378	62.026	1.00	64.04
	1318	NH1	ARG	690	56.283	-1.533	62.029	1.00	58.19
55	1319	NH2	ARG	690	54.427	-0.327	62.623	1.00	62.52
	1320	C	ARG	690	57.274	-3.179	57.177	1.00	57.93
	1321	O	ARG	690	57.037	-1.977	57.067	1.00	59.25
	1322	N	MET	691	58.512	-3.660	57.190	1.00	58.75

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1323	CA	MET	691	59.664	-2.783	57.048	1.00	64.96
1324	CB	MET	691	60.928	-3.542	57.450	1.00	61.53
1325	CG	MET	691	62.247	-3.016	56.886	1.00	59.40
1326	SD	MET	691	62.942	-4.201	55.673	1.00	61.45
1327	CE	MET	691	63.225	-5.669	56.764	1.00	60.93
1328	C	MET	691	59.775	-2.254	55.621	1.00	61.68
1329	O	MET	691	60.130	-1.099	55.405	1.00	63.95
1330	N	THR	692	59.459	-3.097	54.646	1.00	59.70
1331	CA	THR	692	59.519	-2.698	53.243	1.00	60.57
1332	CB	THR	692	59.105	-3.855	52.323	1.00	62.51
1333	OG1	THR	692	59.796	-5.046	52.714	1.00	59.90
1334	CG2	THR	692	59.437	-3.523	50.879	1.00	60.93
1335	C	THR	692	58.586	-1.523	52.962	1.00	60.46
1336	O	THR	692	58.890	-0.655	52.143	1.00	59.04
1337	N	TYR	693	57.439	-1.516	53.634	1.00	61.66
1338	CA	TYR	693	56.459	-0.458	53.461	1.00	60.32
1339	CB	TYR	693	55.045	-1.033	53.553	1.00	59.81
1340	CG	TYR	693	54.665	-1.802	52.302	1.00	61.04
1341	CD1	TYR	693	54.552	-1.153	51.073	1.00	63.46
1342	CE1	TYR	693	54.292	-1.865	49.909	1.00	65.96
1343	CD2	TYR	693	54.497	-3.185	52.332	1.00	59.82
1344	CE2	TYR	693	54.236	-3.906	51.170	1.00	63.54
1345	CZ	TYR	693	54.137	-3.242	49.967	1.00	62.96
1346	OH	TYR	693	53.901	-3.961	48.822	1.00	59.68
1347	C	TYR	693	56.663	0.664	54.458	1.00	58.94
1348	O	TYR	693	55.877	1.600	54.527	1.00	59.49
1349	N	ILE	694	57.720	0.555	55.248	1.00	63.16
1350	CA	ILE	694	58.052	1.598	56.195	1.00	61.35
1351	CB	ILE	694	58.734	1.042	57.462	1.00	59.89
1352	CG2	ILE	694	59.652	2.101	58.077	1.00	62.13
1353	CG1	ILE	694	57.668	0.580	58.457	1.00	63.95
1354	CD1	ILE	694	58.216	0.168	59.793	1.00	61.57
1355	C	ILE	694	59.028	2.478	55.430	1.00	58.86
1356	O	ILE	694	58.989	3.701	55.541	1.00	62.76
1357	N	LYS	695	59.890	1.838	54.643	1.00	61.80
1358	CA	LYS	695	60.869	2.539	53.821	1.00	60.19
1359	CB	LYS	695	61.987	1.607	53.364	1.00	61.05

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1360	CG	LYS	695	62.768	0.892	54.438	1.00	60.54
	1361	CD	LYS	695	63.876	0.081	53.767	1.00	63.44
	1362	CE	LYS	695	64.516	-0.947	54.699	1.00	61.61
10	1363	NZ	LYS	695	65.330	-1.962	53.942	1.00	62.18
	1364	C	LYS	695	60.206	3.074	52.559	1.00	61.44
	1365	O	LYS	695	60.706	4.010	51.946	1.00	61.23
15	1366	N	GLU	696	59.101	2.452	52.156	1.00	61.65
	1367	CA	GLU	696	58.381	2.862	50.961	1.00	60.70
	1368	CB	GLU	696	57.289	1.851	50.635	1.00	62.74
20	1369	CG	GLU	696	56.806	1.901	49.200	1.00	63.74
	1370	CD	GLU	696	57.927	1.725	48.187	1.00	63.24
	1371	OE1	GLU	696	58.903	1.002	48.494	1.00	61.23
25	1372	OE2	GLU	696	57.824	2.299	47.079	1.00	62.98
	1373	C	GLU	696	57.775	4.215	51.260	1.00	61.27
	1374	O	GLU	696	57.594	5.051	50.366	1.00	61.63
30	1375	N	LEU	697	57.468	4.414	52.540	1.00	59.99
	1376	CA	LEU	697	56.912	5.668	53.022	1.00	63.89
	1377	CB	LEU	697	56.314	5.493	54.418	1.00	58.18
35	1378	CG	LEU	697	55.831	6.810	55.016	1.00	62.97
	1379	CD1	LEU	697	54.754	7.370	54.127	1.00	59.80
	1380	CD2	LEU	697	55.319	6.606	56.425	1.00	59.24
40	1381	C	LEU	697	58.029	6.709	53.072	1.00	61.66
	1382	O	LEU	697	57.807	7.871	52.774	1.00	60.35
	1383	N	GLY	698	59.228	6.283	53.460	1.00	59.57
45	1384	CA	GLY	698	60.348	7.198	53.523	1.00	61.15
	1385	C	GLY	698	60.570	7.770	52.146	1.00	60.91
	1386	O	GLY	698	60.748	8.977	51.988	1.00	61.15
50	1387	N	LYS	699	60.557	6.880	51.156	1.00	60.97
	1388	CA	LYS	699	60.729	7.219	49.745	1.00	60.90
	1389	CB	LYS	699	60.526	5.983	48.875	1.00	66.06
55	1390	CG	LYS	699	61.729	5.098	48.621	1.00	61.25
	1391	CD	LYS	699	61.290	3.930	47.737	1.00	59.41
	1392	CE	LYS	699	62.371	3.498	46.765	1.00	61.62
	1393	NZ	LYS	699	63.066	2.246	47.178	1.00	60.87
	1394	C	LYS	699	59.710	8.256	49.289	1.00	58.54
	1395	O	LYS	699	60.019	9.127	48.482	1.00	59.98
	1396	N	ALA	700	58.483	8.128	49.777	1.00	63.02

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1397	CA	ALA	700	57.423	9.048	49.408	1.00	61.82
1398	CB	ALA	700	56.094	8.540	49.926	1.00	65.26
1399	C	ALA	700	57.712	10.422	49.977	1.00	60.36
1400	O	ALA	700	57.545	11.434	49.298	1.00	62.77
1401	N	ILE	701	58.137	10.446	51.235	1.00	65.16
1402	CA	ILE	701	58.471	11.683	51.917	1.00	64.84
1403	CB	ILE	701	58.931	11.406	53.338	1.00	61.36
1404	CG2	ILE	701	59.509	12.670	53.953	1.00	63.03
1405	CG1	ILE	701	57.761	10.874	54.151	1.00	61.61
1406	CD1	ILE	701	58.167	10.364	55.495	1.00	60.05
1407	C	ILE	701	59.574	12.455	51.195	1.00	61.64
1408	O	ILE	701	59.597	13.683	51.228	1.00	58.62
1409	N	VAL	702	60.500	11.749	50.555	1.00	63.95
1410	CA	VAL	702	61.560	12.438	49.831	1.00	57.69
1411	CB	VAL	702	62.815	11.532	49.665	1.00	63.59
1412	CG1	VAL	702	63.310	11.093	51.024	1.00	59.75
1413	CG2	VAL	702	62.494	10.330	48.819	1.00	64.22
1414	C	VAL	702	61.038	12.907	48.466	1.00	61.62
1415	O	VAL	702	61.328	14.014	48.031	1.00	61.64
1416	N	LYS	703	60.244	12.065	47.814	1.00	61.58
1417	CA	LYS	703	59.666	12.387	46.516	1.00	60.75
1418	CB	LYS	703	58.475	11.474	46.201	1.00	56.80
1419	CG	LYS	703	57.419	12.161	45.293	1.00	59.93
1420	CD	LYS	703	55.967	11.815	45.660	1.00	60.60
1421	CE	LYS	703	54.962	12.848	45.088	1.00	57.15
1422	NZ	LYS	703	55.070	13.064	43.605	1.00	62.62
1423	C	LYS	703	59.169	13.814	46.392	1.00	61.49
1424	O	LYS	703	59.454	14.472	45.404	1.00	58.34
1425	N	ARG	704	58.390	14.271	47.367	1.00	63.00
1426	CA	ARG	704	57.826	15.621	47.321	1.00	60.60
1427	CB	ARG	704	56.331	15.590	47.661	1.00	62.95
1428	CG	ARG	704	56.026	15.010	49.033	1.00	61.71
1429	CD	ARG	704	54.728	15.553	49.548	1.00	60.30
1430	NE	ARG	704	54.931	16.417	50.702	1.00	62.33
1431	CZ	ARG	704	53.983	17.200	51.204	1.00	60.19
1432	NH1	ARG	704	52.784	17.213	50.640	1.00	61.68
1433	NH2	ARG	704	54.225	17.965	52.263	1.00	63.26

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1434	C	ARG	704	58.520	16.607	48.249	1.00	63.14
	1435	O	ARG	704	58.732	17.772	47.885	1.00	60.41
	1436	N	GLU	705	58.842	16.155	49.458	1.00	60.89
10	1437	CA	GLU	705	59.528	17.018	50.412	1.00	62.58
	1438	CB	GLU	705	59.814	16.288	51.730	1.00	60.91
	1439	CG	GLU	705	58.605	16.091	52.605	1.00	62.30
15	1440	CD	GLU	705	57.847	17.384	52.817	1.00	64.22
	1441	OE1	GLU	705	56.684	17.460	52.347	1.00	58.55
	1442	OE2	GLU	705	58.419	18.317	53.440	1.00	61.42
20	1443	C	GLU	705	60.848	17.456	49.801	1.00	62.10
	1444	O	GLU	705	61.869	16.761	49.939	1.00	59.78
	1445	N	GLY	706	60.823	18.597	49.115	1.00	60.22
25	1446	CA	GLY	706	62.036	19.100	48.500	1.00	61.75
	1447	C	GLY	706	63.159	19.239	49.518	1.00	60.44
	1448	O	GLY	706	64.168	18.519	49.450	1.00	61.54
30	1449	N	ASN	707	62.974	20.148	50.477	1.00	61.06
	1450	CA	ASN	707	63.989	20.387	51.491	1.00	60.61
	1451	CB	ASN	707	63.561	21.505	52.443	1.00	63.06
35	1452	CG	ASN	707	64.731	22.048	53.258	1.00	60.50
	1453	OD1	ASN	707	64.663	23.152	53.803	1.00	61.18
	1454	ND2	ASN	707	65.815	21.269	53.342	1.00	61.75
40	1455	C	ASN	707	64.355	19.143	52.281	1.00	61.56
	1456	O	ASN	707	63.685	18.767	53.250	1.00	63.56
	1457	N	SER	708	65.446	18.525	51.837	1.00	62.02
45	1458	CA	SER	708	66.024	17.326	52.427	1.00	60.22
	1459	CB	SER	708	67.379	17.070	51.737	1.00	58.91
	1460	OG	SER	708	68.112	15.998	52.305	1.00	62.15
50	1461	C	SER	708	66.200	17.500	53.945	1.00	63.60
	1462	O	SER	708	66.754	16.635	54.624	1.00	60.95
	1463	N	SER	709	65.713	18.619	54.474	1.00	61.83
55	1464	CA	SER	709	65.826	18.922	55.894	1.00	61.35
	1465	CB	SER	709	66.279	20.373	56.065	1.00	65.65
	1466	OG	SER	709	67.479	20.615	55.332	1.00	62.14
	1467	C	SER	709	64.516	18.684	56.641	1.00	59.54
	1468	O	SER =	709	64.497	18.583	57.874	1.00	61.29
	1469	N	GLN	710	63.416	18.586	55.900	1.00	62.57
	1470	CA	GLN	710	62.131	18.347	56.533	1.00	61.59

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1471	CB	GLN	710	61.087	19.333	56.007	1.00	58.05
1472	CG	GLN	710	61.469	20.792	56.249	1.00	62.98
1473	CD	GLN	710	60.344	21.776	55.943	1.00	59.84
1474	OE1	GLN	710	59.363	21.882	56.696	1.00	60.97
1475	NE2	GLN	710	60.481	22.502	54.831	1.00	65.14
1476	C	GLN	710	61.683	16.917	56.297	1.00	58.31
1477	O	GLN	710	60.512	16.586	56.466	1.00	60.42
1478	N	ASN	711	62.625	16.063	55.916	1.00	61.21
1479	CA	ASN	711	62.309	14.666	55.673	1.00	63.02
1480	CB	ASN	711	63.407	14.033	54.819	1.00	60.49
1481	CG	ASN	711	63.508	14.675	53.449	1.00	65.80
1482	OD1	ASN	711	62.565	15.303	52.977	1.00	63.88
1483	ND2	ASN	711	64.646	14.507	52.801	1.00	60.91
1484	C	ASN	711	62.090	13.879	56.974	1.00	63.26
1485	O	ASN	711	61.055	13.238	57.155	1.00	58.14
1486	N	TRP	712	63.054	13.930	57.883	1.00	61.93
1487	CA	TRP	712	62.915	13.234	59.148	1.00	59.49
1488	CB	TRP	712	64.259	13.185	59.833	1.00	62.44
1489	CG	TRP	712	65.169	12.333	59.088	1.00	62.60
1490	CD2	TRP	712	65.485	10.980	59.388	1.00	61.74
1491	CE2	TRP	712	66.331	10.516	58.366	1.00	62.04
1492	CE3	TRP	712	65.130	10.108	60.426	1.00	60.92
1493	CD1	TRP	712	65.815	12.637	57.934	1.00	57.10
1494	NE1	TRP	712	66.517	11.552	57.490	1.00	63.63
1495	CZ2	TRP	712	66.832	9.215	58.345	1.00	63.94
1496	CZ3	TRP	712	65.625	8.817	60.407	1.00	65.64
1497	CH2	TRP	712	66.470	8.381	59.370	1.00	62.08
1498	C	TRP	712	61.903	13.954	60.021	1.00	59.14
1499	O	TRP	712	61.372	13.410	60.996	1.00	59.32
1500	N	GLN	713	61.637	15.191	59.640	1.00	60.06
1501	CA	GLN	713	60.705	16.043	60.345	1.00	63.93
1502	CB	GLN	713	60.853	17.455	59.793	1.00	59.11
1503	CG	GLN	713	60.727	18.564	60.802	1.00	61.74
1504	CD	GLN	713	59.352	19.135	60.838	1.00	60.27
1505	OE1	GLN	713	58.660	19.154	59.824	1.00	58.27
1506	NE2	GLN	713	58.942	19.628	61.998	1.00	65.68
1507	C	GLN	713	59.296	15.522	60.107	1.00	57.87

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1508	O	GLN	713	58.472	15.465	61.018	1.00	63.21
	1509	N	ARG	714	59.051	15.125	58.864	1.00	62.15
	1510	CA	ARG	714	57.758	14.626	58.424	1.00	57.88
10	1511	CB	ARG	714	57.668	14.782	56.907	1.00	65.30
	1512	CG	ARG	714	56.272	14.971	56.382	1.00	62.96
	1513	CD	ARG	714	56.301	15.439	54.940	1.00	62.68
15	1514	NE	ARG	714	55.029	15.200	54.267	1.00	62.08
	1515	CZ	ARG	714	53.899	15.828	54.561	1.00	62.26
	1516	NH1	ARG	714	53.877	16.741	55.515	1.00	59.12
20	1517	NH2	ARG	714	52.788	15.535	53.906	1.00	57.33
	1518	C	ARG	714	57.573	13.171	58.831	1.00	60.95
	1519	O	ARG	714	56.531	12.787	59.368	1.00	60.00
25	1520	N	PHE	715	58.594	12.363	58.571	1.00	59.93
	1521	CA	PHE	715	58.551	10.960	58.940	1.00	61.38
	1522	CB	PHE	715	59.934	10.328	58.799	1.00	60.45
30	1523	CG	PHE	715	59.921	8.834	58.843	1.00	63.37
	1524	CD1	PHE	715	59.016	8.119	58.063	1.00	61.57
	1525	CD2	PHE	715	60.824	8.136	59.636	1.00	59.17
35	1526	CE1	PHE	715	59.005	6.732	58.067	1.00	60.07
	1527	CE2	PHE	715	60.824	6.740	59.648	1.00	58.03
	1528	CZ	PHE	715	59.904	6.038	58.856	1.00	61.29
40	1529	C	PHE	715	58.118	10.923	60.394	1.00	61.16
	1530	O	PHE	715	57.409	10.017	60.821	1.00	61.52
	1531	N	TYR	716	58.541	11.925	61.153	1.00	62.10
45	1532	CA	TYR	716	58.178	11.989	62.550	1.00	61.74
	1533	CB	TYR	716	58.962	13.092	63.256	1.00	60.58
	1534	CG	TYR	716	58.729	13.117	64.748	1.00	60.86
50	1535	CD1	TYR	716	59.376	12.213	65.586	1.00	58.32
	1536	CE1	TYR	716	59.159	12.226	66.952	1.00	59.67
	1537	CD2	TYR	716	57.852	14.032	65.318	1.00	60.64
55	1538	CE2	TYR	716	57.625	14.052	66.679	1.00	63.17
	1539	CZ	TYR	716	58.283	13.152	67.493	1.00	58.37
	1540	OH	TYR	716	58.090	13.194	68.856	1.00	59.28
55	1541	C	TYR	716	56.688	12.280	62.662	1.00	61.28
	1542	O	TYR	716	55.952	11.578	63.356	1.00	61.70
	1543	N	GLN	717	56.249	13.318	61.967	1.00	62.49
	1544	CA	GLN	717	54.858	13.716	62.009	1.00	63.77

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1545	CB	GLN	717	54.694	15.061	61.304	1.00	63.18
1546	CG	GLN	717	55.613	16.126	61.888	1.00	62.93
1547	CD	GLN	717	55.418	17.512	61.288	1.00	62.21
1548	OE1	GLN	717	55.545	17.709	60.073	1.00	59.68
1549	NE2	GLN	717	55.125	18.487	62.147	1.00	58.70
1550	C	GLN	717	53.910	12.674	61.426	1.00	61.09
1551	O	GLN	717	52.907	12.338	62.064	1.00	61.62
1552	N	LEU	718	54.228	12.154	60.237	1.00	62.25
1553	CA	LEU	718	53.384	11.144	59.589	1.00	60.93
1554	CB	LEU	718	53.880	10.833	58.166	1.00	61.18
1555	CG	LEU	718	53.823	11.915	57.078	1.00	60.69
1556	CD1	LEU	718	54.322	11.353	55.764	1.00	59.94
1557	CD2	LEU	718	52.411	12.419	56.916	1.00	64.72
1558	C	LEU	718	53.308	9.847	60.391	1.00	61.41
1559	O	LEU	718	52.241	9.270	60.530	1.00	62.27
1560	N	THR	719	54.441	9.387	60.911	1.00	62.60
1561	CA	THR	719	54.469	8.162	61.706	1.00	61.77
1562	CB	THR	719	55.902	7.717	62.001	1.00	63.38
1563	OG1	THR	719	56.590	8.749	62.715	1.00	59.25
1564	CG2	THR	719	56.626	7.420	60.716	1.00	64.41
1565	C	THR	719	53.744	8.362	63.034	1.00	64.18
1566	O	THR	719	53.365	7.398	63.702	1.00	59.43
1567	N	LYS	720	53.562	9.619	63.421	1.00	60.48
1568	CA	LYS	720	52.864	9.913	64.652	1.00	60.21
1569	CB	LYS	720	53.414	11.194	65.281	1.00	63.61
1570	CG	LYS	720	52.661	11.630	66.532	1.00	60.31
1571	CD	LYS	720	52.340	10.450	67.448	1.00	57.45
1572	CE	LYS	720	51.254	10.801	68.472	1.00	57.33
1573	NZ	LYS	720	50.621	9.562	69.037	1.00	61.89
1574	C	LYS	720	51.364	10.023	64.345	1.00	60.76
1575	O	LYS	720	50.523	10.016	65.246	1.00	60.43
1576	N	LEU	721	51.030	10.110	63.061	1.00	65.16
1577	CA	LEU	721	49.634	10.162	62.659	1.00	59.83
1578	CB	LEU	721	49.505	10.724	61.235	1.00	59.18
1579	CG	LEU	721	48.264	11.548	60.867	1.00	63.18
1580	CD1	LEU	721	48.219	11.751	59.366	1.00	62.00
1581	CD2	LEU	721	47.005	10.851	61.327	1.00	62.08

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1582	C	LEU	721	49.163	8.696	62.703	1.00	61.87
	1583	O	LEU	721	48.041	8.405	63.117	1.00	62.35
	1584	N	LEU	722	50.052	7.788	62.282	1.00	62.99
10	1585	CA	LEU	722	49.813	6.339	62.250	1.00	58.34
	1586	CB	LEU	722	50.988	5.635	61.570	1.00	59.92
	1587	CG	LEU	722	51.194	5.933	60.084	1.00	60.23
15	1588	CD1	LEU	722	52.500	5.333	59.636	1.00	58.33
	1589	CD2	LEU	722	50.050	5.373	59.264	1.00	59.18
	1590	C	LEU	722	49.624	5.754	63.651	1.00	62.26
20	1591	O	LEU	722	48.827	4.835	63.860	1.00	60.80
	1592	N	ASP	723	50.389	6.282	64.597	1.00	60.29
	1593	CA	ASP	723	50.321	5.870	65.989	1.00	61.98
25	1594	CB	ASP	723	51.409	6.583	66.780	1.00	62.74
	1595	CG	ASP	723	52.652	5.759	66.935	1.00	62.09
	1596	OD1	ASP	723	52.840	4.814	66.146	1.00	62.64
30	1597	OD2	ASP	723	53.445	6.066	67.848	1.00	60.13
	1598	C	ASP	723	48.970	6.275	66.554	1.00	61.71
	1599	O	ASP	723	48.281	5.496	67.202	1.00	61.64
35	1600	N	SER	724	48.612	7.524	66.305	1.00	62.20
	1601	CA	SER	724	47.362	8.090	66.784	1.00	61.12
	1602	CB	SER	724	47.329	9.579	66.449	1.00	63.08
40	1603	OG	SER	724	47.513	9.767	65.057	1.00	61.03
	1604	C	SER	724	46.098	7.419	66.246	1.00	59.27
	1605	O	SER	724	45.015	7.664	66.772	1.00	61.79
45	1606	N	MET	725	46.229	6.594	65.203	1.00	60.63
	1607	CA	MET	725	45.077	5.893	64.615	1.00	60.05
	1608	CB	MET	725	45.425	5.228	63.272	1.00	60.16
50	1609	CG	MET	725	45.452	6.151	62.055	1.00	66.62
	1610	SD	MET	725	43.992	7.180	61.838	1.00	58.95
	1611 1	CE	MET	725	42.904	6.134	61.000	1.00	61.36
55	1612	C	MET	725	44.573	4.833	65.576	1.00	64.25
	1613	O	MET	725	43.382	4.543	65.627	1.00	59.89
	1614	N	HIS	726	45.492	4.251	66.334	1.00	62.22
55	1615	CA	HIS	726	45.122	3.249	67.313	1.00	60.86
	1616	CB	HIS	726	46.356	2.746	68.064	1.00	58.90
	1617	CG	HIS	726	47.183	1.772	67.286	1.00	59.73
	1618	CD2	HIS	726	48.518	1.706	67.070	1.00	60.15

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1619	ND1	HIS	726	46.635	0.682	66.646	1.00	61.70
1620	CE1	HIS	726	47.598	-0.014	66.069	1.00	61.05
1621	NE2	HIS	726	48.750	0.586	66.311	1.00	60.76
1622	C	HIS	726	44.141	3.880	68.291	1.00	61.09
1623	O	HIS	726	43.146	3.268	68.650	1.00	60.43
1624	N	GLU	727	44.425	5.109	68.714	1.00	61.91
1625	CA	GLU	727	43.548	5.825	69.642	1.00	58.28
1626	CB	GLU	727	44.218	7.109	70.159	1.00	63.92
1627	CG	GLU	727	43.254	8.102	70.846	1.00	59.43
1628	CD	GLU	727	43.073	9.413	70.053	1.00	61.79
1629	OE1	GLU	727	44.079	10.150	69.874	1.00	60.96
1630	OE2	GLU	727	41.931	9.707	69.607	1.00	63.98
1631	C	GLU	727	42.220	6.187	68.993	1.00	60.97
1632	O	GLU	727	41.163	6.009	69.596	1.00	58.72
1633	N	VAL	728	42.263	6.699	67.769	1.00	60.50
1634	CA	VAL	728	41.022	7.073	67.105	1.00	60.74
1635	CB	VAL	728	41.289	7.922	65.828	1.00	58.90
1636	CG1	VAL	728	42.719	7.804	65.415	1.00	58.73
1637	CG2	VAL	728	40.382	7.494	64.703	1.00	65.58
1638	C	VAL	728	40.192	5.842	66.773	1.00	59.91
1639	O	VAL	728	38.971	5.844	66.931	1.00	61.17
1640	N	VAL	729	40.872	4.792	66.326	1.00	61.77
1641	CA	VAL	729	40.243	3.522	65.974	1.00	62.39
1642	CB	VAL	729	41.277	2.578	65.332	1.00	60.27
1643	CG1	VAL	729	40.946	1.131	65.606	1.00	61.53
1644	CG2	VAL	729	41.298	2.815	63.866	1.00	60.01
1645	C	VAL	729	39.586	2.830	67.173	1.00	61.69
1646	O	VAL	729	38.718	1.971	67.009	1.00	59.65
1647	N	GLU	730	39.999	3.199	68.377	1.00	59.90
1648	CA	GLU	730	39.411	2.601	69.558	1.00	60.27
1649	CB	GLU	730	40.308	2.812	70.755	1.00	59.45
1650	CG	GLU	730	39.878	2.014	71.942	1.00	66.48
1651	CD	GLU	730	40.681	2.348	73.167	1.00	62.84
1652 -	OE1	GLU	730	41.912	2.547	73.039	1.00	61.03
1653	OE2	GLU	730	40.081	2.400	74.263	1.00	60.34
1654	C	GLU	730	38.085	3.291	69.804	1.00	62.24
1655	O	GLU	730	37.031	2.660	69.869	1.00	60.10

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1656	N	ASN	731	38.154	4.606	69.941	1.00	61.01
	1657	CA	ASN	731	36.967	5.409	70.157	1.00	60.41
	1658	CB	ASN	731	37.356	6.880	70.212	1.00	62.98
10	1659	CG	ASN	731	37.593	7.333	71.613	1.00	59.54
	1660	OD1	ASN	731	36.657	7.385	72.410	1.00	58.59
	1661	ND2	ASN	731	38.841	7.638	71.945	1.00	58.18
15	1662	C	ASN	731	35.917	5.165	69.081	1.00	61.30
	1663	O	ASN	731	34.720	5.345	69.317	1.00	60.95
	1664	N	LEU	732	36.364	4.750	67.902	1.00	60.39
20	1665	CA	LEU	732	35.442	4.475	66.820	1.00	61.55
	1666	CB	LEU	732	36.141	4.550	65.471	1.00	59.24
	1667	CG	LEU	732	36.184	5.931	64.813	1.00	64.00
25	1668	CD1	LEU	732	36.712	5.787	63.374	1.00	62.90
	1669	CD2	LEU	732	34.771	6.561	64.818	1.00	60.26
	1670	C	LEU	732	34.841	3.108	66.997	1.00	60.27
30	1671	O	LEU	732	33.648	2.922	66.774	1.00	61.79
	1672	N	LEU	733	35.673	2.148	67.399	1.00	58.72
	1673	CA	LEU	733	35.214	0.770	67.612	1.00	60.63
35	1674	CB	LEU	733	36.376	-0.153	67.969	1.00	60.85
	1675	CG	LEU	733	37.087	-0.798	66.782	1.00	56.83
	1676	CD1	LEU	733	38.344	-1.474	67.266	1.00	63.66
40	1677	CD2	LEU	733	36.159	-1.786	66.083	1.00	56.09
	1678	C	LEU	733	34.158	0.663	68.696	1.00	60.11
	1679	O	LEU	733	33.092	0.098	68.458	1.00	60.20
45	1680	N	ASN	734	34.456	1.192	69.883	1.00	64.88
	1681	CA	ASN	734	33.503	1.148	70.988	1.00	60.87
	1682	CB	ASN	734	33.874	2.130	72.099	1.00	64.42
50	1683	CG	ASN	734	35.076	1.683	72.896	1.00	60.85
	1684	OD1	ASN	734	35.499	0.526	72.817	1.00	60.20
	1685	ND2	ASN	734	35.627	2.597	73.686	1.00	62.04
55	1686	C	ASN	734	32.157	1.544	70.455	1.00	59.98
	1687	O	ASN	734	31.209	0.755	70.478	1.00	59.10
	1688	N	TYR	735	32.085	2.778	69.969	1.00	61.85
55	1689	CA	TYR	735	30.844	3.294	69.421	1.00	63.27
	1690	CB	TYR	735	31.075	4.640	68.743	1.00	60.68
	1691	CG	TYR	735	29.867	5.515	68.853	1.00	62.56
	1692	CD1	TYR	735	28.777	5.328	67.975	1.00	60.84

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1693	CE1	TYR	735	27.586	6.030	68.168	1.00	60.10
1694	CD2	TYR	735	29.722	6.421	69.889	1.00	62.93
1695	CE2	TYR	735	28.543	7.127	70.084	1.00	62.59
1696	CZ	TYR	735	27.483	6.916	69.221	1.00	60.99
1697	OH	TYR	735	26.305	7.561	69.418	1.00	56.15
1698	C	TYR	735	30.261	2.306	68.418	1.00	57.10
1699	O	TYR	735	29.052	2.158	68.321	1.00	60.19
1700	N	CYS	736	31.126	1.621	67.682	1.00	62.53
1701	CA	CYS	736	30.673	0.644	66.707	1.00	60.21
1702	CB	CYS	736	31.842	0.208	65.815	1.00	62.29
1703	SG	CYS	736	31.461	-1.142	64.660	1.00	62.77
1704	C	CYS	736	30.063	-0.572	67.399	1.00	62.99
1705	O	CYS	736	28.857	-0.795	67.290	1.00	61.76
1706	N	PHE	737	30.892	-1.346	68.111	1.00	60.76
1707	CA	PHE	737	30.435	-2.546	68.835	1.00	61.61
1708	CB	PHE	737	31.454	-3.013	69.889	1.00	65.67
1709	CG	PHE	737	32.718	-3.575	69.321	1.00	61.17
1710	CD1	PHE	737	32.732	-4.173	68.069	1.00	62.43
1711	CD2	PHE	737	33.904	-3.515	70.049	1.00	62.09
1712	CE1	PHE	737	33.908	-4.704	67.544	1.00	60.80
1713	CE2	PHE	737	35.083	-4.042	69.536	1.00	61.51
1714	CZ	PHE	737	35.086	-4.638	68.279	1.00	59.32
1715	C	PHE	737	29.151	-2.266	69.581	1.00	60.98
1716	O	PHE	737	28.103	-2.865	69.312	1.00	61.98
1717	N	GLN	738	29.274	-1.356	70.542	1.00	64.21
1718	CA	GLN	738	28.183	-0.934	71.399	1.00	63.22
1719	CB	GLN	738	28.613	0.301	72.173	1.00	64.29
1720	CG	GLN	738	27.542	0.896	73.021	1.00	59.02
1721	CD	GLN	738	27.555	2.392	72.920	1.00	61.20
1722	OE1	GLN	738	27.116	2.962	71.916	1.00	60.80
1723	NE2	GLN	738	28.082	3.048	73.948	1.00	57.12
1724	C	GLN	738	26.917	-0.640	70.606	1.00	61.18
1725	O	GLN	738	25.827	-1.017	71.009	1.00	61.34
1726	N	THR	739	27.056	0.037	69.478	1.00	61.45
1727	CA	THR	739	25.893	0.326	68.678	1.00	60.85
1728	CB	THR	739	26.208	1.297	67.542	1.00	55.90
1729	OG1	THR	739	26.212	2.649	68.047	1.00	60.51

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1730	CG2	THR	739	25.193	1.200	66.444	1.00	62.24
	1731	C	THR	739	25.330	-0.969	68.085	1.00	62.53
	1732	O	THR	739	24.122	-1.107	67.898	1.00	60.85
10	1733	N	PHE	740	26.221	-1.906	67.784	1.00	61.25
	1734	CA	PHE	740	25.859	-3.197	67.215	1.00	59.86
	1735	CB	PHE	740	27.110	-3.854	66.641	1.00	60.28
15	1736	CG	PHE	740	26.937	-5.301	66.311	1.00	63.82
	1737	CD1	PHE	740	26.434	-5.690	65.079	1.00	62.86
	1738	CD2	PHE	740	27.297	-6.278	67.236	1.00	61.71
20	1739	CE1	PHE	740	26.295	-7.042	64.763	1.00	60.86
	1740	CE2	PHE	740	27.165	-7.623	66.938	1.00	60.83
	1741	CZ	PHE	740	26.663	-8.013	65.696	1.00	60.77
25	1742	C	PHE	740	25.200	-4.140	68.238	1.00	60.76
	1743	O	PHE	740	24.420	-5.028	67.866	1.00	60.72
	1744	N	LEU	741	25.538	-3.965	69.515	1.00	62.82
30	1745	CA	LEU	741	24.976	-4.793	70.584	1.00	61.57
	1746	CB	LEU	741	25.991	-5.012	71.708	1.00	59.14
	1747	CG	LEU	741	27.187	-5.904	71.404	1.00	62.48
35	1748	CD1	LEU	741	28.083	-5.956	72.627	1.00	58.13
	1749	CD2	LEU	741	26.708	-7.294	71.021	1.00	60.31
	1750	C	LEU	741	23.770	-4.087	71.165	1.00	60.19
40	1751	O	LEU	741	23.577	-4.055	72.389	1.00	59.64
	1752	N	ASP	742	22.960	-3.508	70.290	1.00	61.92
	1753	CA	ASP	742	21.789	-2.797	70.762	1.00	60.22
45	1754	CB	ASP	742	22.185	-1.372	71.179	1.00	61.70
	1755	CG	ASP	742	21.021	-0.598	71.793	1.00	60.82
	1756	OD1	ASP	742	21.258	0.438	72.473	1.00	60.77
50	1757	OD2	ASP	742	19.863	-1.028	71.587	1.00	61.09
	1758	C	ASP	742	20.689	-2.769	69.710	1.00	61.90
	1759	O	ASP	742	20.530	-1.782	68.995	1.00	61.23
55	1760	N	LYS	743	19.934	-3.864	69.623	1.00	63.29
	1761	CA	LYS	743	18.833	-3.975	68.664	1.00	62.18
	1762	CB	LYS	743	18.045	-5.273	68.888	1.00	63.55
	1763	CG	LYS	743	18.054	-6.243	67.705	1.00	62.77
	1764	CD	LYS	743	17.301	-5.691	66.489	1.00	59.38
	1765	CE	LYS	743	17.291	-6.724	65.349	1.00	62.80
	1766	NZ	LYS	743	16.446	-6.335	64.166	1.00	57.45

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
1767	C	LYS	743	17.899	-2.786	68.822	1.00	62.93
1768	O	LYS	743	17.407	-2.248	67.833	1.00	58.22
1769	N	THR	744	17.669	-2.383	70.069	1.00	61.23
1770	CA	THR	744	16.808	-1.247	70.400	1.00	61.48
1771	CB	THR	744	17.148	-0.715	71.802	1.00	63.18
1772	OG1	THR	744	17.199	-1.817	72.719	1.00	59.84
1773	CG2	THR	744	16.112	0.308	72.265	1.00	60.98
1774	C	THR	744	16.913	-0.077	69.411	1.00	59.67
1775	O	THR	744	15.913	0.580	69.118	1.00	64.20
1776	N	MET	745	18.117	0.184	68.903	1.00	61.36
1777	CA	MET	745	18.322	1.282	67.961	1.00	62.05
1778	CB	MET	745	19.703	1.909	68.158	1.00	63.01
1779	CG	MET	745	20.029	2.189	69.614	1.00	61.21
1780	SD	MET	745	21.418	3.324	69.877	1.00	62.14
1781	CE	MET	745	20.934	4.087	71.538	1.00	61.78
1782	C	MET	745	18.175	0.824	66.517	1.00	59.56
1783	O	MET	745	18.382	1.605	65.585	1.00	62.58
1784	N	SER	746	17.817	-0.442	66.334	1.00	59.78
1785	CA	SER	746	17.624	-1.000	64.996	1.00	58.09
1786	CB	SER	746	16.169	-0.786	64.541	1.00	58.34
1787	OG	SER	746	15.252	-1.368	65.455	1.00	63.83
1788	C	SER	746	18.592	-0.429	63.940	1.00	59.09
1789	O	SER	746	18.176	0.027	62.867	1.00	61.57
1790	N	ILE	747	19.882	-0.432	64.269	1.00	62.10
1791	CA	ILE	747	20.905	0.022	63.342	1.00	61.22
1792	CB	ILE	747	22.021	0.814	64.054	1.00	63.05
1793	CG2	ILE	747	23.241	0.930	63.145	1.00	64.60
1794	CG1	ILE	747	21.499	2.205	64.426	1.00	61.38
1795	CD1	ILE	747	22.576	3.198	64.804	1.00	63.35
1796	C	ILE	747	21.465	-1.260	62.749	1.00	62.54
1797	O	ILE	747	22.169	-2.011	63.419	1.00	60.09
1798	N	GLU	748	21.125	-1.507	61.491	1.00	60.25
1799	CA	GLU	748	21.541	-2.711	60.787	1.00	60.97
1800	CB	GLU	748	20.497	-3.038	59.709	1.00	63.45
1801	CG	GLU	748	20.877	-4.168	58.756	1.00	60.81
1802	CD	GLU	748	19.678	-4.723	57.973	1.00	59.13
1803	OE1	GLU	748	19.013	-3.932	57.262	1.00	62.39

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1804	OE2	GLU	748	19.406	-5.950	58.072	1.00	61.13
	1805	C	GLU	748	22.940	-2.658	60.175	1.00	61.28
	1806	O	GLU	748	23.391	-1.616	59.690	1.00	62.62
10	1807	N	PHE	749	23.622	-3.800	60.231	1.00	62.73
	1808	CA	PHE	749	24.963	-3.959	59.667	1.00	59.35
	1809	CB	PHE	749	25.974	-4.421	60.733	1.00	59.45
15	1810	CG	PHE	749	26.299	-3.389	61.759	1.00	64.74
	1811	CD1	PHE	749	25.399	-3.085	62.770	1.00	59.18
	1812	CD2	PHE	749	27.514	-2.721	61.721	1.00	57.96
20	1813	CE1	PHE	749	25.708	-2.119	63.742	1.00	61.52
	1814	CE2	PHE	749	27.839	-1.753	62.685	1.00	65.31
	1815	CZ	PHE	749	26.934	-1.451	63.697	1.00	59.87
25	1816	C	PHE	749	24.872	-5.048	58.599	1.00	60.75
	1817	O	PHE	749	24.047	-5.952	58.705	1.00	62.03
	1818	N	PRO	750	25.705	-4.970	57.550	1.00	61.23
30	1819	CD	PRO	750	26.645	-3.910	57.166	1.00	60.04
	1820	CA	PRO	750	25.652	-6.003	56.516	1.00	61.34
	1821	CB	PRO	750	26.584	-5.468	55.434	1.00	64.04
35	1822	CG	PRO	750	26.608	-4.015	55.668	1.00	60.17
	1823	C	PRO	750	26.240	-7.235	57.172	1.00	60.83
	1824	O	PRO	750	26.788	-7.143	58.271	1.00	59.53
40	1825	N	GLU	751	26.139	-8.386	56.523	1.00	60.43
	1826	CA	GLU	751	26.719	-9.572	57.122	1.00	61.33
	1827	CB	GLU	751	26.350	-10.834	56.311	1.00	62.90
45	1828	CG	GLU	751	25.560	-10.608	55.002	1.00	60.51
	1829	CD	GLU	751	26.436	-10.142	53.837	1.00	57.86
	1830	OE1	GLU	751	27.420	-10.844	53.519	1.00	60.97
50	1831	OE2	GLU	751	26.138	-9.084	53.240	1.00	59.16
	1832	C	GLU	751	28.255	-9.389	57.219	1.00	58.48
	1833	O	GLU	751	28.850	-9.561	58.292	1.00	59.47
55	1834	N	MET	752	28.891	-9.004	56.115	1.00	64.26
	1835	CA	MET	752	30.336	-8.808	56.109	1.00	61.15
	1836	CB	MET	752	30.777	-8.060	54.857	1.00	63.84
60	1837	CG	MET	752	32.255	-7.666	54.898	1.00	64.44
	1838	SD	MET	752	33.383	-9.076	55.043	1.00	67.15
	1839	CE	MET	752	33.649	-9.386	53.307	1.00	59.96
65	1840	C	MET	752	30.884	-8.072	57.323	1.00	62.38

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1841	O	MET	752	31.963	-8.394	57.811	1.00	60.81
	1842	N	LEU	753	30.163	-7.067	57.796	1.00	59.19
	1843	CA	LEU	753	30.627	-6.323	58.957	1.00	62.39
10	1844	CB	LEU	753	30.187	-4.862	58.881	1.00	61.65
	1845	CG	LEU	753	31.214	-3.835	58.397	1.00	61.49
	1846	CD1	LEU	753	31.713	-4.171	57.010	1.00	61.11
	1847	CD2	LEU	753	30.567	-2.471	58.411	1.00	63.29
15	1848	C	LEU	753	30.114	-6.946	60.241	1.00	58.84
	1849	O	LEU	753	30.779	-6.885	61.273	1.00	61.39
	1850	N	ALA	754	28.927	-7.541	60.177	1.00	62.56
20	1851	CA	ALA	754	28.337	-8.194	61.343	1.00	61.99
	1852	CB	ALA	754	26.963	-8.775	60.983	1.00	59.37
	1853	C	ALA	754	29.287	-9.313	61.747	1.00	66.01
	1854	O	ALA	754	29.619	-9.482	62.922	1.00	63.54
25	1855	N	GLU	755	29.724	-10.044	60.722	1.00	63.92
	1856	CA	GLU	755	30.632	-11.194	60.795	1.00	59.42
	1857	CB	GLU	755	30.674	-11.851	59.407	1.00	60.24
30	1858	CG	GLU	755	31.733	-12.933	59.190	1.00	62.29
	1859	CD	GLU	755	31.348	-14.260	59.811	1.00	59.60
	1860	OE1	GLU	755	30.318	-14.834	59.388	1.00	60.67
	1861	OE2	GLU	755	32.075	-14.728	60.719	1.00	62.46
35	1862	C	GLU	755	32.068	-10.912	61.252	1.00	60.75
	1863	O	GLU	755	32.906	-11.809	61.240	1.00	61.42
	1864	N	ILE	756	32.363	-9.677	61.636	1.00	60.43
40	1865	CA	ILE	756	33.709	-9.328	62.074	1.00	65.41
	1866	CB	ILE	756	34.369	-8.336	61.114	1.00	58.24
	1867	CG2	ILE	756	35.741	-7.964	61.623	1.00	57.70
	1868	CG1	ILE	756	34.478	-8.957	59.729	1.00	59.57
45	1869	CD1	ILE	756	35.178	-8.090	58.743	1.00	61.24
	1870	C	ILE	756	33.625	-8.693	63.439	1.00	63.18
	1871	O	ILE	756	34.373	-9.043	64.351	1.00	58.77
50	1872	N	ILE	757	32.705	-7.740	63.548	1.00	59.89
	1873	CA	ILE	757	32.434	-7.024	64.785	1.00	61.90
	1874	CB	ILE	757	31.115	-6.254	64.668	1.00	64.77
	1875	CG2	ILE	757	30.778	-5.602	65.991	1.00	62.61
55	1876	CG1	ILE	757	31.224	-5.237	63.529	1.00	62.60
	1877	CD1	ILE	757	29.902	-4.649	63.097	1.00	59.02

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1878	C	ILE	757	32.298	-8.069	65.879	1.00	60.76
	1879	O	ILE	757	32.990	-8.016	66.890	1.00	60.98
	1880	N	THR	758	31.396	-9.022	65.660	1.00	59.72
10	1881	CA	THR	758	31.184	-10.104	66.608	1.00	61.21
	1882	CB	THR	758	30.224	-11.141	66.017	1.00	58.63
	1883	OG1	THR	758	30.260	-11.028	64.592	1.00	60.88
15	1884	CG2	THR	758	28.792	-10.925	66.527	1.00	60.75
	1885	C	THR	758	32.540	-10.770	66.885	1.00	61.53
	1886	O	THR	758	33.167	-10.549	67.926	1.00	61.44
20	1887	N	ASN	759	32.979	-11.572	65.924	1.00	62.04
	1888	CA	ASN	759	34.240	-12.305	65.965	1.00	60.58
	1889	CB	ASN	759	34.426	-13.001	64.623	1.00	60.54
25	1890	CG	ASN	759	33.242	-12.774	63.689	1.00	60.06
	1891	OD1	ASN	759	32.581	-11.723	63.736	1.00	59.27
	1892	ND2	ASN	759	32.976	-13.747	62.825	1.00	59.97
30	1893	C	ASN	759	35.470	-11.432	66.249	1.00	59.08
	1894	O	ASN	759	36.564	-11.710	65.734	1.00	63.02
	1895	N	GLN	760	35.282	-10.388	67.059	1.00	60.43
35	1896	CA	GLN	760	36.336	-9.442	67.438	1.00	61.43
	1897	CB	GLN	760	36.620	-8.446	66.302	1.00	56.98
	1898	CG	GLN	760	37.445	-8.966	65.121	1.00	61.31
40	1899	CD	GLN	760	38.839	-9.446	65.514	1.00	63.88
	1900	OE1	GLN	760	39.445	-8.949	66.463	1.00	59.43
	1901	NE2	GLN	760	39.356	-10.409	64.769	1.00	62.96
45	1902	C	GLN	760	35.850	-8.659	68.651	1.00	59.31
	1903	O	GLN	760	36.625	-8.353	69.563	1.00	59.88
	1904	N	ILE	761	34.546	-8.371	68.649	1.00	61.08
50	1905	CA	ILE	761	33.861	-7.606	69.704	1.00	64.40
	1906	CB	ILE	761	32.318	-7.582	69.469	1.00	60.77
	1907	CG2	ILE	761	31.759	-8.983	69.575	1.00	61.46
55	1908	CG1	ILE	761	31.626	-6.686	70.500	1.00	61.86
	1909	CD1	ILE	761	30.115	-6.703	70.390	1.00	62.34
	1910	C	ILE	761	34.111	-8.077	71.139	1.00	63.06
55	1911	O	ILE	761	33.900	-7.317	72.087	1.00	60.11
	1912	N	PRO	762	34.543	-9.338	71.319	1.00	58.19
	1913	CD	PRO	762	34.581	-10.454	70.353	1.00	61.52
	1914	CA	PRO	762	34.800	-9.840	72.670	1.00	60.05

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	1915	CB	PRO	762	34.718	-11.350	72.482	1.00	60.47
	1916	CG	PRO	762	35.309	-11.528	71.122	1.00	62.98
	1917	C	PRO	762	36.160	-9.419	73.230	1.00	59.07
	1918	O	PRO	762	36.257	-8.697	74.232	1.00	61.15
10	1919	N	LYS	763	37.203	-9.887	72.558	1.00	59.41
	1920	CA	LYS	763	38.580	-9.637	72.960	1.00	61.27
	1921	CB	LYS	763	39.424	-10.882	72.594	1.00	61.66
15	1922	CG	LYS	763	40.926	-10.651	72.347	1.00	62.08
	1923	CD	LYS	763	41.206	-9.910	71.025	1.00	58.99
	1924	CE	LYS	763	40.834	-10.723	69.776	1.00	60.53
	1925	NZ	LYS	763	39.378	-11.026	69.623	1.00	62.94
20	1926	C	LYS	763	39.256	-8.359	72.438	1.00	63.01
	1927	O	LYS	763	40.164	-7.846	73.086	1.00	63.43
	1928	N	TYR	764	38.820	-7.847	71.289	1.00	64.75
25	1929	CA	TYR	764	39.428	-6.653	70.673	1.00	58.42
	1930	CB	TYR	764	38.399	-5.865	69.876	1.00	62.63
	1931	CG	TYR	764	38.901	-5.590	68.486	1.00	65.16
30	1932	CD1	TYR	764	38.708	-6.516	67.467	1.00	57.96
	1933	CE1	TYR	764	39.190	-6.287	66.180	1.00	61.30
	1934	CD2	TYR	764	39.600	-4.422	68.192	1.00	61.22
	1935	CE2	TYR	764	40.092	-4.183	66.902	1.00	61.36
35	1936	CZ	TYR	764	39.876	-5.118	65.901	1.00	59.50
	1937	OH	TYR	764	40.304	-4.863	64.612	1.00	62.78
	1938	C	TYR	764	40.204	-5.654	71.535	1.00	61.96
40	1939	O	TYR	764	41.310	-5.963	72.003	1.00	61.04
	1940	N	SER	765	39.653	-4.443	71.701	1.00	60.29
	1941	CA	SER	765	40.324	-3.419	72.519	1.00	61.03
45	1942	CB	SER	765	39.780	-1.999	72.208	1.00	57.40
	1943	OG	SER	765	38.359	-1.934	72.144	1.00	59.00
	1944	C	SER	765	40.207	-3.760	74.016	1.00	59.80
	1945	O	SER	765	39.574	-3.046	74.809	1.00	60.59
50	1946	N	ASN	766	40.833	-4.884	74.371	1.00	59.36
	1947	CA	ASN	766	40.867	-5.404	75.738	1.00	63.02
	1948	CB	ASN	766	40.390	-6.867	75.745	1.00	59.32
	1949	CG	ASN	766	38.959	-7.018	75.239	1.00	61.45
55	1950	OD1	ASN	766	38.593	-6.456	74.197	1.00	60.60
	1951	ND2	ASN	766	38.143	-7.782	75.971	1.00	64.82

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	1952	C	ASN	766	42.301	-5.305	76.311	1.00	62.76
	1953	O	ASN	766	42.503	-4.889	77.469	1.00	60.59
	1954	N	GLY	767	43.281	-5.673	75.478	1.00	59.11
10	1955	CA	GLY	767	44.689	-5.653	75.860	1.00	59.91
	1956	C	GLY	767	45.366	-6.867	75.232	1.00	61.75
	1957	O	GLY	767	46.588	-6.912	75.041	1.00	61.17
15	1958	N	ASN	768	44.532	-7.846	74.887	1.00	62.80
	1959	CA	ASN	768	44.942	-9.109	74.276	1.00	62.46
	1960	CB	ASN	768	43.717	-10.032	74.246	1.00	59.72
20	1961	CG	ASN	768	42.798	-9.832	75.467	1.00	60.42
	1962	OD1	ASN	768	41.697	-10.404	75.538	1.00	59.89
	1963	ND2	ASN	768	43.248	-9.020	76.427	1.00	63.45
25	1964	C	ASN	768	45.543	-8.940	72.855	1.00	63.10
	1965	O	ASN	768	46.095	-9.882	72.282	1.00	62.80
	1966	N	ILE	769	45.418	-7.744	72.284	1.00	58.10
30	1967	CA	ILE	769	45.984	-7.464	70.967	1.00	60.18
	1968	CB	ILE	769	45.006	-6.713	70.036	1.00	61.64
	1969	CG2	ILE	769	45.569	-6.703	68.614	1.00	59.97
35	1970	CG1	ILE	769	43.623	-7.361	70.051	1.00	65.54
	1971	CD1	ILE	769	42.605	-6.626	69.175	1.00	65.14
	1972	C	ILE	769	47.192	-6.544	71.150	1.00	59.44
40	1973	O	ILE	769	47.217	-5.701	72.058	1.00	61.97
	1974	N	LYS	770	48.175	-6.692	70.267	1.00	61.57
	1975	CA	LYS	770	49.391	-5.890	70.314	1.00	60.09
45	1976	CB	LYS	770	50.601	-6.778	70.033	1.00	61.51
	1977	CG	LYS	770	51.961	-6.172	70.339	1.00	61.08
	1978	CD	LYS	770	53.041	-7.224	70.047	1.00	59.40
50	1979	CE	LYS	770	54.344	-6.982	70.801	1.00	62.15
	1980	NZ	LYS	770	55.339	-8.089	70.604	1.00	63.19
	1981	C	LYS	770	49.333	-4.776	69.277	1.00	63.90
55	1982	O	LYS	770	49.439	-5.031	68.071	1.00	62.08
	1983	N	LYS	771	49.161	-3.545	69.754	1.00	59.06
	1984	CA	LYS	771	49.103	-2.376	68.884	1.00	61.08
55	1985	CB	LYS	771	48.386	-1.212	69.589	1.00	63.15
	1986	CG	LYS	771	49.188	-0.525	70.712	1.00	63.84
	1987	CD	LYS	771	48.443	0.681	71.308	1.00	63.12
	1988	CE	LYS	771	49.384	1.588	72.100	1.00	59.83

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	1989	NZ	LYS	771	48.821	2.970	72.186	1.00	60.16
	1990	C	LYS	771	50.532	-1.976	68.550	1.00	60.42
	1991	O	LYS	771	51.276	-1.561	69.430	1.00	62.03
10	1992	N	LEU	772	50.928	-2.120	67.290	1.00	60.80
	1993	CA	LEU	772	52.285	-1.756	66.890	1.00	58.97
	1994	CB	LEU	772	52.629	-2.368	65.533	1.00	62.77
15	1995	CG	LEU	772	52.781	-3.885	65.492	1.00	63.82
	1996	CD1	LEU	772	52.780	-4.346	64.046	1.00	62.61
	1997	CD2	LEU	772	54.071	-4.295	66.203	1.00	63.11
20	1998	C	LEU	772	52.405	-0.243	66.812	1.00	61.57
	1999	O	LEU	772	51.513	0.428	66.289	1.00	60.62
	2000	N	LEU	773	53.499	0.296	67.341	1.00	59.76
25	2001	CA	LEU	773	53.704	1.734	67.317	1.00	60.00
	2002	CB	LEU	773	53.602	2.320	68.725	1.00	59.66
	2003	CG	LEU	773	52.221	2.321	69.380	1.00	62.80
30	2004	CD1	LEU	773	52.290	2.999	70.729	1.00	61.23
	2005	CD2	LEU	773	51.233	3.053	68.490	1.00	65.68
	2006	C	LEU	773	55.051	2.094	66.727	1.00	62.80
35	2007	O	LEU	773	55.911	1.234	66.517	1.00	61.81
	2008	N	PHE	774	55.219	3.382	66.456	1.00	60.94
	2009	CA	PHE	774	56.451	3.917	65.897	1.00	61.49
40	2010	CB	PHE	774	56.128	4.864	64.743	1.00	63.45
	2011	CG	PHE	774	55.889	4.169	63.451	1.00	61.20
	2012	CD1	PHE	774	56.936	3.532	62.802	1.00	63.76
45	2013	CD2	PHE	774	54.621	4.105	62.902	1.00	61.89
	2014	CE1	PHE	774	56.727	2.838	61.627	1.00	56.93
	2015	CE2	PHE	774	54.395	3.409	61.720	1.00	59.92
50	2016	CZ	PHE	774	55.451	2.773	61.081	1.00	62.56
	2017	C	PHE	774	57.175	4.681	66.984	1.00	60.20
	2018	O	PHE	774	58.400	4.702	67.046	1.00	60.03
55	2019	N	HIS	775	56.384	5.301	67.849	1.00	62.48
	2020	CA	HIS	775	56.905	6.104	68.934	1.00	64.64
	2021	CB	HIS	775	56.466	7.558	68.730	1.00	61.69
	2022	CG	HIS	775	56.898	8.120	67.417	1.00	59.70
	2023	CD2	HIS	775	56.188	8.565	66.356	1.00	62.49
	2024	ND1	HIS	775	58.223	8.191	67.047	1.00	60.30
	2025	CE1	HIS	775	58.313	8.652	65.813	1.00	59.19

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2063	C	ASN	743	34.842	-16.318	58.192	1.00	60.80
2064	O	ASN	743	35.780	-16.196	57.410	1.00	62.67
2065	N	ALA	744	33.779	-17.075	57.935	1.00	59.69
2066	CA	ALA	744	33.640	-17.827	56.696	1.00	61.76
2067	CB	ALA	744	32.350	-18.623	56.729	1.00	60.04
2068	C	ALA	744	33.675	-16.930	55.453	1.00	62.63
2069	O	ALA	744	34.423	-17.199	54.503	1.00	58.54
2070	N	LEU	745	32.869	-15.866	55.462	1.00	60.19
2071	CA	LEU	745	32.820	-14.936	54.329	1.00	62.12
2072	CB	LEU	745	31.855	-13.783	54.617	1.00	60.59
2073	CG	LEU	745	30.606	-13.726	53.739	1.00	58.63
2074	CD1	LEU	745	29.895	-12.400	53.937	1.00	64.25
2075	CD2	LEU	745	31.004	-13.902	52.291	1.00	60.41
2076	C	LEU	745	34.190	-14.360	53.952	1.00	61.72
2077	O	LEU	745	34.521	-14.276	52.776	1.00	59.83
2078	N	LEU	746	34.978	-13.961	54.946	1.00	57.79
2079	CA	LEU	746	36.311	-13.413	54.691	1.00	60.45
2080	CB	LEU	746	36.898	-12.849	55.989	1.00	61.06
2081	CG	LEU	746	37.673	-11.534	55.956	1.00	61.13
2082	CD1	LEU	746	38.380	-11.374	57.275	1.00	61.70
2083	CD2	LEU	746	38.664	-11.520	54.823	1.00	61.56
2084	C	LEU	746	37.249	-14.511	54.156	1.00	58.73
2085	O	LEU	746	37.905	-14.356	53.120	1.00	62.68
2086	N	ARG	747	37.307	-15.613	54.895	1.00	61.00
2087	CA	ARG	747	38.145	-16.759	54.560	1.00	57.24
2088	CB	ARG	747	37.853	-17.906	55.539	1.00	66.74
2089	CG	ARG	747	38.332	-19.278	55.102	1.00	61.05
2090	CD	ARG	747	38.533	-20.190	56.319	1.00	62.51
2091	NE	ARG	747	39.807	-19.938	56.998	1.00	62.06
2092	CZ	ARG	747	39.952	-19.867	58.321	1.00	63.78
2093	NH1	ARG	747	38.894	-20.023	59.118	1.00	60.31
2094	NH2	ARG	747	41.156	-19.637	58.848	1.00	60.80
2095	C	ARG	747	37.883	-17.186	53.134	1.00	59.12
2096	O	ARG	747	38.793	-17.589	52.418	1.00	62.02
2097	N	TYR	748	36.623	-17.088	52.731	1.00	61.89
2098	CA	TYR	748	36.215	-17.449	51.387	1.00	65.00
2099	CB	TYR	748	34.685	-17.413	51.301	1.00	58.95

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2100	CG	TYR	748	34.136	-17.350	49.897	1.00	62.12
	2101	CD1	TYR	748	34.256	-18.429	49.021	1.00	63.79
	2102	CE1	TYR	748	33.805	-18.342	47.715	1.00	61.69
10	2103	CD2	TYR	748	33.544	-16.185	49.430	1.00	61.63
	2104	CE2	TYR	748	33.091	-16.084	48.127	1.00	60.08
	2105	CZ	TYR	748	33.226	-17.163	47.272	1.00	58.42
15	2106	OH	TYR	748	32.806	-17.030	45.966	1.00	59.74
	2107	C	TYR	748	36.832	-16.447	50.419	1.00	61.75
	2108	O	TYR	748	37.599	-16.807	49.532	1.00	61.82
20	2109	N	LEU	749	36.501	-15.178	50.628	1.00	60.52
	2110	CA	LEU	749	36.974	-14.069	49.800	1.00	61.53
	2111	CB	LEU	749	36.380	-12.757	50.303	1.00	63.00
25	2112	CG	LEU	749	34.873	-12.741	50.535	1.00	57.09
	2113	CD1	LEU	749	34.508	-11.427	51.167	1.00	62.85
	2114	CD2	LEU	749	34.113	-12.954	49.233	1.00	62.37
30	2115	C	LEU	749	38.482	-13.910	49.733	1.00	64.05
	2116	O	LEU	749	38.991	-13.275	48.807	1.00	61.97
	2117	N	LEU	750	39.195	-14.475	50.703	1.00	59.99
35	2118	CA	LEU	750	40.644	-14.363	50.728	1.00	63.11
	2119	CB	LEU	750	41.147	-14.497	52.167	1.00	62.65
	2120	CG	LEU	750	41.463	-13.160	52.849	1.00	63.02
40	2121	CD1	LEU	750	41.695	-13.344	54.327	1.00	58.04
	2122	CD2	LEU	750	42.693	-12.559	52.194	1.00	62.24
	2123	C	LEU	750	41.436	-15.294	49.803	1.00	64.30
45	2124	O	LEU	750	42.666	-15.246	49.796	1.00	58.24
	2125	N	ASP	751	40.745	-16.129	49.024	1.00	59.30
	2126	CA	ASP	751	41.396	-17.048	48.068	1.00	62.49
50	2127	CB	ASP	751	41.860	-18.337	48.764	1.00	62.90
	2128	CG	ASP	751	40.921	-18.784	49.855	1.00	62.09
	2129	OD1	ASP	751	40.342	-17.900	50.526	1.00	62.68
55	2130	OD2	ASP	751	40.779	-20.014	50.051	1.00	60.33
	2131	C	ASP	751	40.472	-17.371	46.897	1.00	61.25
	2132	O	ASP	751	39.476	-18.065	47.053	1.00	61.96
	2133	N	LYS	752	40.824	-16.849	45.725	1.00	62.34
	2134	CA	LYS	752	40.030	-17.003	44.506	1.00	62.50
	2135	CB	LYS	752	38.733	-16.160	44.600	1.00	63.17
	2136	CG	LYS	752	37.872	-16.386	45.858	1.00	60.82

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2137	CD	LYS	752	36.923	-15.230	46.159	1.00	62.16
2138	CE	LYS	752	35.726	-15.186	45.223	1.00	60.30
2139	NZ	LYS	752	36.101	-15.095	43.779	1.00	61.47
2140	C	LYS	752	40.895	-16.438	43.384	1.00	63.98
2141	O	LYS	752	42.043	-16.833	43.212	1.00	60.08
2142	N	ASP	753	40.322	-15.496	42.641	1.00	61.50
2143	CA	ASP	753	41.004	-14.809	41.552	1.00	60.87
2144	CB	ASP	753	41.969	-13.778	42.151	1.00	61.81
2145	CG	ASP	753	41.293	-12.886	43.212	1.00	65.36
2146	OD1	ASP	753	40.845	-13.417	44.262	1.00	58.98
2147	OD2	ASP	753	41.204	-11.653	42.996	1.00	62.40
2148	C	ASP	753	41.712	-15.723	40.533	1.00	62.25
2149	O	ASP	753	41.905	-16.929	40.770	1.00	62.51
2150	N	ASP	754	42.076	-15.125	39.394	1.00	59.26
2151	CA	ASP	754	42.713	-15.818	38.271	1.00	62.08
2152	CB	ASP	754	42.118	-15.302	36.949	1.00	60.51
2153	CG	ASP	754	41.121	-14.148	37.150	1.00	60.95
2154	OD1	ASP	754	40.683	-13.555	36.135	1.00	61.57
2155	OD2	ASP	754	40.762	-13.831	38.304	1.00	61.61
2156	C	ASP	754	44.236	-15.678	38.234	1.00	60.21
2157	O	ASP	754	44.946	-16.712	38.264	1.00	63.29
2158	OXT	ASP	754	44.707	-14.526	38.169	1.00	61.39
2159	CB	GLN	527	44.425	43.308	57.458	1.00	59.84
2160	CG	GLN	527	45.330	43.181	58.697	1.00	63.06
2161	CD	GLN	527	46.173	41.895	58.675	1.00	61.64
2162	OE1	GLN	527	46.913	41.596	59.623	1.00	62.44
2163	NE2	GLN	527	46.065	41.137	57.583	1.00	63.46
2164	C	GLN	527	43.994	44.763	55.475	1.00	60.61
2165	O	GLN	527	44.711	45.517	54.798	1.00	61.62
2166	N	GLN	527	42.843	45.238	57.671	1.00	62.80
2167	CA	GLN	527	44.095	44.745	57.006	1.00	60.11
2168	N	LEU	528	43.105	43.912	54.955	1.00	62.93
2169	CA	LEU	528	42.857	43.747	53.516	1.00	58.92
2170	CB	LEU	528	43.696	42.579	52.979	1.00	61.24
2171	CG	LEU	528	45.210	42.751	53.124	1.00	58.97
2172	CD1	LEU	528	45.858	41.410	53.501	1.00	57.95
2173	CD2	LEU	528	45.778	43.371	51.831	1.00	60.61

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2174	C	LEU	528	41.369	43.449	53.303	1.00	63.94
	2175	O	LEU	528	40.531	44.290	53.650	1.00	62.36
	2176	N	THR	529	41.067	42.256	52.748	1.00	59.95
10	2177	CA	THR	529	39.689	41.769	52.487	1.00	61.84
	2178	CB	THR	529	39.396	40.430	53.232	1.00	59.05
	2179	OG1	THR	529	40.375	39.442	52.866	1.00	63.83
15	2180	CG2	THR	529	37.997	39.920	52.882	1.00	59.80
	2181	C	THR	529	38.725	42.842	52.992	1.00	61.32
	2182	O	THR	529	37.988	42.645	53.973	1.00	61.35
20	2183	N	PRO	530	38.704	43.977	52.271	1.00	64.25
	2184	CD	PRO	530	38.650	43.494	50.878	1.00	59.35
	2185	CA	PRO	530	38.021	45.276	52.317	1.00	58.74
25	2186	CB	PRO	530	37.610	45.502	50.860	1.00	60.27
	2187	CG	PRO	530	37.368	44.132	50.384	1.00	65.84
	2188	C	PRO	530	36.839	45.387	53.239	1.00	62.92
30	2189	O	PRO	530	36.948	45.328	54.474	1.00	60.28
	2190	N	THR	531	35.706	45.591	52.590	1.00	63.85
	2191	CA	THR	531	34.443	45.708	53.246	1.00	62.34
35	2192	CB	THR	531	34.253	47.135	53.851	1.00	63.80
	2193	OG1	THR	531	33.854	47.016	55.230	1.00	64.25
	2194	CG2	THR	531	33.218	47.940	53.067	1.00	61.34
40	2195	C	THR	531	33.526	45.410	52.081	1.00	61.78
	2196	O	THR	531	32.505	44.758	52.251	1.00	61.93
	2197	N	LEU	532	33.917	45.822	50.877	1.00	62.02
45	2198	CA	LEU	532	33.060	45.545	49.722	1.00	60.94
	2199	CB	LEU	532	33.410	46.445	48.528	1.00	57.32
	2200	CG	LEU	532	32.463	46.285	47.329	1.00	64.49
50	2201	CD1	LEU	532	31.027	46.313	47.771	1.00	61.90
	2202	CD2	LEU	532	32.702	47.377	46.344	1.00	62.84
	2203	C	LEU	532	33.077	44.077	49.283	1.00	61.37
55	2204	O	LEU	532	32.016	43.461	49.149	1.00	62.65
	2205	N	VAL	533	34.266	43.518	49.052	1.00	61.22
	2206	CA	VAL	533	34.366	42.119	48.635	1.00	60.75
55	2207	CB	VAL	533	35.781	41.753	48.114	1.00	59.58
	2208	CG1	VAL	533	36.697	41.400	49.264	1.00	60.31
	2209	CG2	VAL	533	35.695	40.576	47.185	1.00	59.77
	2210	C	VAL	533	34.062	41.240	49.840	1.00	63.61

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2211	O	VAL	533	33.861	40.038	49.709	1.00	62.93
2212	N	SER	534	34.053	41.859	51.013	1.00	61.64
2213	CA	SER	534	33.774	41.170	52.260	1.00	60.61
2214	CB	SER	534	34.143	42.089	53.425	1.00	62.32
2215	OG	SER	534	34.391	41.364	54.612	1.00	60.70
2216	C	SER	534	32.276	40.880	52.270	1.00	62.67
2217	O	SER	534	31.799	39.906	52.854	1.00	59.90
2218	N	LEU	535	31.544	41.747	51.593	1.00	60.18
2219	CA	LEU	535	30.102	41.644	51.508	1.00	60.75
2220	CB	LEU	535	29.527	42.975	51.048	1.00	61.59
2221	CG	LEU	535	28.027	43.101	51.245	1.00	61.16
2222	CD1	LEU	535	27.773	43.835	52.537	1.00	63.92
2223	CD2	LEU	535	27.416	43.850	50.089	1.00	61.72
2224	C	LEU	535	29.688	40.547	50.543	1.00	60.18
2225	O	LEU	535	28.852	39.714	50.868	1.00	58.39
2226	N	LEU	536	30.269	40.552	49.349	1.00	60.57
2227	CA	LEU	536	29.950	39.536	48.355	1.00	63.14
2228	CB	LEU	536	30.813	39.719	47.115	1.00	61.69
2229	CG	LEU	536	30.671	40.980	46.284	1.00	63.99
2230	CD1	LEU	536	31.622	40.864	45.118	1.00	60.60
2231	CD2	LEU	536	29.247	41.145	45.801	1.00	62.81
2232	C	LEU	536	30.204	38.140	48.908	1.00	61.72
2233	O	LEU	536	29.703	37.141	48.379	1.00	60.04
2234	N	GLU	537	30.996	38.086	49.970	1.00	60.48
2235	CA	GLU	537	31.359	36.838	50.607	1.00	61.60
2236	CB	GLU	537	32.691	37.003	51.307	1.00	61.56
2237	CG	GLU	537	33.169	35.763	51.998	1.00	58.70
2238	CD	GLU	537	34.599	35.907	52.442	1.00	62.52
2239	OE1	GLU	537	35.173	34.900	52.919	1.00	61.18
2240	OE2	GLU	537	35.140	37.033	52.305	1.00	60.21
2241	C	GLU	537	30.344	36.288	51.592	1.00	59.30
2242	O	GLU	537	30.094	35.084	51.604	1.00	60.22
2243	N	VAL	538	29.773	37.155	52.424	1.00	61.88
2244	CA	VAL	538	28.781	36.714	53.399	1.00	62.81
2245	CB	VAL	538	28.636	37.687	54.591	1.00	57.08
2246	CG1	VAL	538	29.993	38.283	54.957	1.00	61.43
2247	CG2	VAL	538	27.611	38.757	54.268	1.00	60.61

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2248	C	VAL	538	27.420	36.586	52.752	1.00	61.99
	2249	O	VAL	538	26.576	35.841	53.233	1.00	61.89
	2250	N	ILE	539	27.203	37.322	51.669	1.00	61.34
10	2251	CA	ILE	539	25.931	37.263	50.977	1.00	60.88
	2252	CB	ILE	539	25.628	38.548	50.209	1.00	57.53
	2253	CG2	ILE	539	26.034	39.737	51.035	1.00	63.74
15	2254	CG1	ILE	539	26.365	38.550	48.869	1.00	64.95
	2255	CD1	ILE	539	25.847	39.584	47.898	1.00	61.40
	2256	C	ILE	539	25.946	36.133	49.977	1.00	59.86
20	2257	O	ILE	539	24.984	35.934	49.251	1.00	60.95
	2258	N	GLU	540	27.051	35.408	49.919	1.00	61.19
	2259	CA	GLU	540	27.170	34.290	48.993	1.00	64.61
25	2260	CB	GLU	540	28.620	33.798	48.960	1.00	61.89
	2261	CG	GLU	540	28.917	32.628	48.022	1.00	59.99
	2262	CD	GLU	540	28.635	32.926	46.560	1.00	60.98
30	2263	OE1	GLU	540	28.949	34.050	46.103	1.00	60.19
	2264	OE2	GLU	540	28.113	32.025	45.861	1.00	58.09
	2265	C	GLU	540	26.241	33.181	49.469	1.00	60.25
35	2266	O	GLU	540	26.357	32.710	50.603	1.00	62.79
	2267	N	PRO	541	25.289	32.766	48.614	1.00	59.70
	2268	CD	PRO	541	24.961	33.287	47.275	1.00	61.01
40	2269	CA	PRO	541	24.362	31.703	49.013	1.00	61.09
	2270	CB	PRO	541	23.361	31.665	47.861	1.00	63.13
	2271	CG	PRO	541	24.138	32.177	46.694	1.00	57.00
45	2272	C	PRO	541	25.051	30.365	49.254	1.00	60.83
	2273	O	PRO	541	25.979	29.988	48.535	1.00	60.28
	2274	N	GLU	542	24.607	29.669	50.297	1.00	60.82
50	2275	CA	GLU	542	25.157	28.364	50.655	1.00	61.11
	2276	CB	GLU	542	24.607	27.933	52.001	1.00	63.94
	2277	CG	GLU	542	23.163	27.558	51.899	1.00	65.51
55	2278	CD	GLU	542	22.569	27.217	53.237	1.00	61.20
	2279	OE1	GLU	542	21.369	26.813	53.269	1.00	64.82
	2280	OE2	GLU	542	23.307	27.360	54.253	1.00	61.05
	2281	C	GLU	542	24.668	27.393	49.584	1.00	60.85
	2282	O	GLU	542	23.631	27.637	48.966	1.00	61.52
	2283	N	VAL	543	25.369	26.291	49.353	1.00	62.89
	2284	CA	VAL	543	24.879	25.397	48.316	1.00	61.20

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2285	CB	VAL	543	26.029	24.589	47.676	1.00	60.15
2286	CG1	VAL	543	27.366	25.164	48.116	1.00	61.25
2287	CG2	VAL	543	25.903	23.132	48.011	1.00	64.25
2288	C	VAL	543	23.745	24.465	48.760	1.00	61.19
2289	O	VAL	543	23.506	24.232	49.955	1.00	61.59
2290	N	LEU	544	23.037	23.944	47.769	1.00	60.75
2291	CA	LEU	544	21.910	23.068	48.018	1.00	62.70
2292	CB	LEU	544	20.686	23.557	47.244	1.00	61.76
2293	CG	LEU	544	20.315	25.041	47.237	1.00	62.21
2294	CD1	LEU	544	19.968	25.490	48.639	1.00	60.39
2295	CD2	LEU	544	21.464	25.856	46.654	1.00	61.37
2296	C	LEU	544	22.209	21.639	47.591	1.00	61.62
2297	O	LEU	544	23.047	21.388	46.721	1.00	61.82
2298	N	TYR	545	21.504	20.713	48.222	1.00	60.41
2299	CA	TYR	545	21.623	19.306	47.915	1.00	64.14
2300	CB	TYR	545	21.436	18.495	49.189	1.00	59.96
2301	CG	TYR	545	22.566	18.713	50.160	1.00	66.69
2302	CD1	TYR	545	22.715	17.908	51.287	1.00	63.31
2303	CE1	TYR	545	23.810	18.056	52.122	1.00	61.54
2304	CD2	TYR	545	23.537	19.684	49.907	1.00	62.21
2305	CE2	TYR	545	24.632	19.843	50.739	1.00	61.49
2306	CZ	TYR	545	24.769	19.022	51.842	1.00	59.50
2307	OH	TYR	545	25.898	19.142	52.619	1.00	60.93
2308	C	TYR	545	20.482	19.111	46.949	1.00	58.64
2309	O	TYR	545	19.553	19.912	46.956	1.00	62.56
2310	N	ALA	546	20.532	18.077	46.115	1.00	57.51
2311	CA	ALA	546	19.461	17.886	45.145	1.00	59.14
2312	CB	ALA	546	20.026	17.390	43.845	1.00	60.50
2313	C	ALA	546	18.347	16.965	45.595	1.00	62.16
2314	O	ALA	546	17.352	16.821	44.895	1.00	62.38
2315	N	GLY	547	18.493	16.338	46.755	1.00	59.60
2316	CA	GLY	547	17.441	15.445	47.203	1.00	63.46
2317	C	GLY	547	17.125	14.408	46.137	1.00	63.02
2318	O	GLY	547	15.968	14.068	45.890	1.00	60.60
2319	N	TYR	548	18.180	13.918	45.496	1.00	62.10
2320	CA	TYR	548	18.095	12.906	44.447	1.00	60.16
2321	CB	TYR	548	19.366	12.971	43.621	1.00	60.58

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2322	CG	TYR	548	19.357	12.107	42.403	1.00	61.55
	2323	CD1	TYR	548	18.522	12.406	41.331	1.00	65.33
	2324	CE1	TYR	548	18.550	11.657	40.175	1.00	62.35
10	2325	CD2	TYR	548	20.218	11.023	42.292	1.00	62.44
	2326	CE2	TYR	548	20.251	10.267	41.142	1.00	64.59
	2327	CZ	TYR	548	19.416	10.594	40.086	1.00	60.42
15	2328	OH	TYR	548	19.467	9.877	38.925	1.00	60.60
	2329	C	TYR	548	17.979	11.519	45.080	1.00	60.53
	2330	O	TYR	548	18.584	11.272	46.114	1.00	61.95
20	2331	N	ASP	549	17.227	10.603	44.480	1.00	60.31
	2332	CA	ASP	549	17.135	9.281	45.088	1.00	60.89
	2333	CB	ASP	549	16.206	8.359	44.317	1.00	61.64
25	2334	CG	ASP	549	15.653	7.256	45.196	1.00	62.87
	2335	OD1	ASP	549	16.437	6.715	45.997	1.00	61.92
	2336	OD2	ASP	549	14.446	6.929	45.100	1.00	58.12
30	2337	C	ASP	549	18.525	8.656	45.152	1.00	62.05
	2338	O	ASP	549	19.176	8.728	46.190	1.00	59.43
	2339	N	SER	550	18.977	8.052	44.049	1.00	61.36
35	2340	CA	SER	550	20.312	7.425	43.963	1.00	61.16
	2341	CB	SER	550	21.301	8.127	44.910	1.00	61.33
	2342	OG	SER	550	22.637	8.055	44.435	1.00	65.58
40	2343	C	SER	550	20.286	5.923	44.268	1.00	62.72
	2344	O	SER	550	21.025	5.138	43.662	1.00	61.37
	2345	N	SER	551	19.422	5.543	45.206	1.00	60.55
45	2346	CA	SER	551	19.262	4.155	45.623	1.00	62.47
	2347	CB	SER	551	18.461	4.092	46.927	1.00	59.78
	2348	OG	SER	551	17.138	4.551	46.727	1.00	65.75
50	2349	C	SER	551	18.548	3.348	44.544	1.00	61.26
	2350	O	SER	551	18.187	2.189	44.749	1.00	64.05
	2351	N	VAL	552	18.349	3.976	43.394	1.00	61.88
55	2352	CA	VAL	552	17.683	3.338	42.268	1.00	61.07
	2353	CB	VAL	552	16.146	3.536	42.346	1.00	61.01
	2354	CG1	VAL	552	15.781	4.362	43.582	1.00	62.13
55	2355	CG2	VAL	552	15.642	4.194	41.084	1.00	63.59
	2356	C	VAL	552	18.245	3.935	40.975	1.00	60.74
	2357	O	VAL	552	18.423	5.151	40.872	1.00	60.94
	2358	N	PRO	553	18.502	3.085	39.966	1.00	57.88

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2359	CD	PRO	553	17.755	1.824	39.869	1.00	60.27
2360	CA	PRO	553	19.058	3.418	38.648	1.00	60.29
2361	CB	PRO	553	18.407	2.387	37.718	1.00	59.38
2362	CG	PRO	553	17.208	1.918	38.478	1.00	59.68
2363	C	PRO	553	18.933	4.837	38.105	1.00	61.75
2364	O	PRO	553	17.864	5.452	38.132	1.00	60.81
2365	N	ASP	554	20.055	5.352	37.616	1.00	59.48
2366	CA	ASP	554	20.061	6.676	37.032	1.00	59.15
2367	CB	ASP	554	21.477	7.212	36.819	1.00	62.17
2368	CG	ASP	554	22.222	7.452	38.101	1.00	62.93
2369	OD1	ASP	554	21.591	7.655	39.164	1.00	60.70
2370	OD2	ASP	554	23.467	7.455	38.017	1.00	60.19
2371	C	ASP	554	19.433	6.505	35.667	1.00	61.49
2372	O	ASP	554	18.898	5.446	35.354	1.00	59.51
2373	N	SER	555	19.536	7.557	34.859	1.00	60.31
2374	CA	SER	555	19.023	7.601	33.492	1.00	60.74
2375	CB	SER	555	17.576	7.113	33.419	1.00	64.15
2376	OG	SER	555	16.687	8.099	33.896	1.00	60.71
2377	C	SER	555	19.092	9.069	33.108	1.00	61.31
2378	O	SER	555	18.776	9.929	33.927	1.00	59.93
2379	N	THR	556	19.525	9.358	31.883	1.00	62.16
2380	CA	THR	556	19.636	10.742	31.434	1.00	61.52
2381	CB	THR	556	19.673	10.857	29.895	1.00	59.01
2382	OG1	THR	556	20.850	10.212	29.391	1.00	60.60
2383	CG2	THR	556	19.677	12.330	29.475	1.00	60.87
2384	C	THR	556	18.422	11.505	31.913	1.00	61.95
2385	O	THR	556	18.517	12.377	32.788	1.00	60.46
2386	N	TRP	557	17.285	11.145	31.318	1.00	60.92
2387	CA	TRP	557	15.986	11.734	31.611	1.00	63.76
2388	CB	TRP	557	14.864	10.739	31.251	1.00	61.57
2389	CG	TRP	557	13.719	10.807	32.225	1.00	57.77
2390	CD2	TRP	557	12.895	11.949	32.491	1.00	60.28
2391	CE2	TRP	557	12.066	11.627	33.595	1.00	61.10
2392	CE3	TRP	557	12.785	13.219	31.911	1.00	57.69
2393	CD1	TRP	557	13.357	9.855	33.145	1.00	63.49
2394	NE1	TRP	557	12.369	10.344	33.974	1.00	60.45
2395	CZ2	TRP	557	11.132	12.535	34.132	1.00	61.64

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2396	CZ3	TRP	557	11.857	14.124	32.452	1.00	61.15
	2397	CH2	TRP	557	11.045	13.773	33.548	1.00	61.06
	2398	C	TRP	557	15.816	12.176	33.063	1.00	61.03
10	2399	O	TRP	557	15.546	13.342	33.335	1.00	63.66
	2400	N	ARG	558	15.972	11.228	33.982	1.00	62.37
	2401	CA	ARG	558	15.798	11.466	35.413	1.00	63.98
15	2402	CB	ARG	558	15.806	10.116	36.134	1.00	61.30
	2403	CG	ARG	558	15.389	10.127	37.590	1.00	62.22
	2404	CD	ARG	558	15.189	8.686	38.070	1.00	59.18
20	2405	NE	ARG	558	16.210	8.204	39.005	1.00	60.75
	2406	CZ	ARG	558	16.280	8.542	40.294	1.00	62.74
	2407	NH1	ARG	558	15.392	9.378	40.820	1.00	65.45
25	2408	NH2	ARG	558	17.222	8.022	41.074	1.00	61.39
	2409	C	ARG	558	16.814	12.416	36.056	1.00	63.08
	2410	O	ARG	558	16.524	13.027	37.085	1.00	62.80
30	2411	N	ILE	559	17.991	12.548	35.451	1.00	63.40
	2412	CA	ILE	559	19.036	13.423	35.983	1.00	59.67
	2413	CB	ILE	559	20.459	12.828	35.701	1.00	59.65
35	2414	CG2	ILE	559	21.437	13.905	35.250	1.00	56.03
	2415	CG1	ILE	559	20.982	12.150	36.968	1.00	58.33
	2416	CD1	ILE	559	22.212	11.327	36.744	1.00	61.31
40	2417	C	ILE	559	18.939	14.862	35.469	1.00	64.14
	2418	O	ILE	559	18.843	15.792	36.281	1.00	63.80
	2419	N	MET	560	18.964	15.060	34.151	1.00	58.15
45	2420	CA	MET	560	18.871	16.419	33.646	1.00	61.08
	2421	CB	MET	560	18.753	16.460	32.095	1.00	60.65
	2422	CG	MET	560	20.117	16.352	31.322	1.00	63.74
50	2423	SD	MET	560	20.038	16.357	29.422	1.00	63.49
	2424	CE	MET	560	21.750	16.939	28.970	1.00	61.12
	2425	C	MET	560	17.634	17.014	34.325	1.00	63.02
55	2426	O	MET	560	17.666	18.156	34.780	1.00	60.37
	2427	N	THR	561	16.572	16.217	34.457	1.00	60.33
	2428	CA	THR	561	15.351	16.677	35.123	1.00	60.71
55	2429	CB	THR	561	14.306	15.540	35.292	1.00	58.90
	2430	OG1	THR	561	14.006	14.959	34.025	1.00	60.27
	2431	CG2	THR	561	13.019	16.080	35.867	1.00	58.67
	2432	C	THR	561	15.616	17.259	36.520	1.00	60.71

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2433	O	THR	561	15.390	18.429	36.747	1.00	62.74
2434	N	THR	562	16.111	16.434	37.451	1.00	61.67
2435	CA	THR	562	16.387	16.821	38.860	1.00	62.60
2436	CB	THR	562	16.914	15.721	39.677	1.00	60.58
2437	OG1	THR	562	18.152	15.292	39.081	1.00	59.96
2438	CG2	THR	562	15.938	14.616	39.802	1.00	62.71
2439	C	THR	562	17.487	17.786	39.098	1.00	60.58
2440	O	THR	562	17.924	18.032	40.229	1.00	63.25
2441	N	LEU	563	17.993	18.325	38.047	1.00	60.71
2442	CA	LEU	563	19.148	19.110	38.123	1.00	61.15
2443	CB	LEU	563	20.009	18.485	37.164	1.00	61.40
2444	CG	LEU	563	21.445	18.268	37.247	1.00	60.76
2445	CD1	LEU	563	21.882	17.094	38.118	1.00	59.56
2446	CD2	LEU	563	21.705	18.012	35.810	1.00	62.29
2447	C	LEU	563	18.542	20.350	37.631	1.00	60.18
2448	O	LEU	563	19.115	21.393	37.453	1.00	62.51
2449	N	ASN	564	17.281	20.194	37.278	1.00	62.12
2450	CA	ASN	564	16.596	21.312	36.741	1.00	63.12
2451	CB	ASN	564	15.703	20.918	35.651	1.00	63.80
2452	CG	ASN	564	16.263	21.124	34.284	1.00	60.00
2453	OD1	ASN	564	17.269	21.801	34.085	1.00	59.72
2454	ND2	ASN	564	15.577	20.559	33.311	1.00	61.08
2455	C	ASN	564	15.740	21.719	37.867	1.00	61.56
2456	O	ASN	564	15.204	22.818	37.863	1.00	61.14
2457	N	MET	565	15.483	20.798	38.768	1.00	63.63
2458	CA	MET	565	14.643	21.083	39.872	1.00	60.96
2459	CB	MET	565	14.164	19.773	40.504	1.00	61.63
2460	CG	MET	565	12.686	19.546	40.369	1.00	65.53
2461	SD	MET	565	12.013	20.320	38.903	1.00	61.09
2462	CE	MET	565	10.337	20.392	39.357	1.00	60.22
2463	C	MET	565	15.560	21.814	40.802	1.00	62.76
2464	O	MET	565	15.162	22.713	41.539	1.00	60.13
2465	N	LEU	566	16.826	21.447	40.746	1.00	62.63
2466	CA	LEU	566	17.794	22.101	41.590	1.00	58.73
2467	CB	LEU	566	19.007	21.188	41.764	1.00	59.94
2468	CG	LEU	566	20.381	21.435	42.410	1.00	60.09
2469	CD1	LEU	566	21.236	21.209	41.243	1.00	60.52

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2470	CD2	LEU	566	20.687	22.805	43.045	1.00	59.08
	2471	C	LEU	566	18.142	23.418	40.952	1.00	61.33
	2472	O	LEU	566	18.373	24.398	41.652	1.00	61.14
10	2473	N	GLY	567	18.140	23.461	39.625	1.00	57.88
	2474	CA	GLY	567	18.436	24.703	38.935	1.00	63.27
	2475	C	GLY	567	17.469	25.785	39.351	1.00	60.49
15	2476	O	GLY	567	17.854	26.938	39.514	1.00	61.62
	2477	N	GLY	568	16.206	25.412	39.526	1.00	63.72
	2478	CA	GLY	568	15.212	26.382	39.936	1.00	60.34
20	2479	C	GLY	568	15.617	27.006	41.256	1.00	60.96
	2480	O	GLY	568	15.913	28.195	41.332	1.00	61.39
	2481	N	ARG	569	15.662	26.196	42.302	1.00	59.63
25	2482	CA	ARG	569	16.011	26.692	43.623	1.00	58.74
	2483	CB	ARG	569	16.143	25.530	44.588	1.00	62.58
	2484	CG	ARG	569	14.860	24.767	44.719	1.00	61.89
30	2485	CD	ARG	569	14.973	23.794	45.842	1.00	60.95
	2486	NE	ARG	569	16.047	22.854	45.573	1.00	60.03
	2487	CZ	ARG	569	16.734	22.229	46.513	1.00	60.68
35	2488	NH1	ARG	569	16.459	22.447	47.793	1.00	65.06
	2489	NH2	ARG	569	17.697	21.391	46.169	1.00	63.36
	2490	C	ARG	569	17.261	27.538	43.671	1.00	59.59
40	2491	O	ARG	569	17.395	28.397	44.539	1.00	58.49
	2492	N	GLN	570	18.179	27.299	42.747	1.00	60.12
	2493	CA	GLN	570	19.417	28.069	42.704	1.00	62.83
45	2494	CB	GLN	570	20.457	27.359	41.852	1.00	64.23
	2495	CG	GLN	570	21.212	26.254	42.529	1.00	60.55
	2496	CD	GLN	570	22.345	25.738	41.674	1.00	61.81
50	2497	OE1	GLN	570	23.046	24.818	42.067	1.00	60.88
	2498	NE2	GLN	570	22.533	26.331	40.499	1.00	56.12
	2499	C	GLN	570	19.195	29.462	42.135	1.00	59.62
55	2500	O	GLN	570	19.872	30.409	42.529	1.00	60.45
	2501	N	VAL	571	18.273	29.571	41.182	1.00	64.99
	2502	CA	VAL	571	17.953	30.851	40.576	1.00	62.98
55	2503	CB	VAL	571	17.141	30.653	39.278	1.00	62.20
	2504	CG1	VAL	571	16.363	31.906	38.929	1.00	61.93
	2505	CG2	VAL	571	18.090	30.312	38.140	1.00	61.13
	2506	C	VAL	571	17.166	31.658	41.605	1.00	63.93

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2507	O	VAL	571	17.379	32.865	41.763	1.00	65.46
2508	N	ILE	572	16.271	30.981	42.317	1.00	61.03
2509	CA	ILE	572	15.483	31.623	43.360	1.00	58.70
2510	CB	ILE	572	14.548	30.605	44.045	1.00	66.72
2511	CG2	ILE	572	14.006	31.169	45.350	1.00	58.22
2512	CG1	ILE	572	13.425	30.220	43.081	1.00	61.85
2513	CD1	ILE	572	12.411	29.251	43.663	1.00	61.02
2514	C	ILE	572	16.456	32.186	44.390	1.00	59.43
2515	O	ILE	572	16.240	33.257	44.948	1.00	61.61
2516	N	ALA	573	17.531	31.446	44.628	1.00	62.51
2517	CA	ALA	573	18.562	31.844	45.571	1.00	63.19
2518	CB	ALA	573	19.467	30.662	45.875	1.00	59.65
2519	C	ALA	573	19.390	32.994	45.016	1.00	60.08
2520	O	ALA	573	19.853	33.852	45.765	1.00	61.27
2521	N	ALA	574	19.573	33.004	43.700	1.00	62.86
2522	CA	ALA	574	20.350	34.039	43.027	1.00	62.91
2523	CB	ALA	574	20.500	33.690	41.553	1.00	60.40
2524	C	ALA	574	19.729	35.426	43.176	1.00	61.54
2525	O	ALA	574	20.402	36.441	42.977	1.00	62.14
2526	N	VAL	575	18.447	35.461	43.535	1.00	63.11
2527	CA	VAL	575	17.721	36.716	43.708	1.00	61.22
2528	CB	VAL	575	16.214	36.502	43.529	1.00	61.11
2529	CG1	VAL	575	15.500	37.835	43.568	1.00	63.45
2530	CG2	VAL	575	15.950	35.795	42.218	1.00	55.96
2531	C	VAL	575	17.970	37.386	45.063	1.00	61.67
2532	O	VAL	575	18.242	38.589	45.119	1.00	61.16
2533	N	LYS	576	17.866	36.618	46.148	1.00	63.44
2534	CA	LYS	576	18.103	37.169	47.477	1.00	61.90
2535	CB	LYS	576	17.913	36.120	48.576	1.00	60.65
2536	CG	LYS	576	16.569	35.385	48.633	1.00	62.95
2537	CD	LYS	576	16.370	34.812	50.045	1.00	61.64
2538	CE	LYS	576	15.453	33.594	50.101	1.00	61.27
2539	NZ	LYS	576	16.134	32.288	49.785	1.00	60.24
2540	C	LYS	576	19.554	37.616	47.498	1.00	62.75
2541	O	LYS	576	19.966	38.384	48.367	1.00	59.51
2542	N	TRP	577	20.320	37.103	46.534	1.00	64.04
2543	CA	TRP	577	21.741	37.407	46.382	1.00	63.24

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2544	CB	TRP	577	22.447	36.277	45.610	1.00	61.04
	2545	CG	TRP	577	23.852	36.613	45.166	1.00	62.92
	2546	CD2	TRP	577	24.285	36.919	43.828	1.00	59.92
10	2547	CE2	TRP	577	25.663	37.212	43.892	1.00	60.22
	2548	CE3	TRP	577	23.637	36.978	42.584	1.00	61.13
	2549	CD1	TRP	577	24.956	36.729	45.958	1.00	63.10
15	2550	NE1	TRP	577	26.045	37.088	45.201	1.00	58.91
	2551	CZ2	TRP	577	26.411	37.557	42.763	1.00	58.75
	2552	CZ3	TRP	577	24.378	37.325	41.461	1.00	63.87
20	2553	CH2	TRP	577	25.754	37.611	41.559	1.00	60.61
	2554	C	TRP	577	21.923	38.719	45.634	1.00	60.28
	2555	O	TRP	577	22.654	39.597	46.083	1.00	61.57
25	2556	N	ALA	578	21.251	38.837	44.490	1.00	60.75
	2557	CA	ALA	578	21.338	40.032	43.661	1.00	62.79
	2558	CB	ALA	578	20.522	39.847	42.395	1.00	63.55
30	2559	C	ALA	578	20.869	41.274	44.409	1.00	60.84
	2560	O	ALA	578	21.347	42.370	44.156	1.00	60.70
	2561	N	LYS	579	19.937	41.105	45.339	1.00	62.74
35	2562	CA	LYS	579	19.423	42.234	46.107	1.00	60.13
	2563	CB	LYS	579	18.016	41.900	46.640	1.00	60.85
	2564	CG	LYS	579	16.969	41.709	45.532	1.00	61.81
40	2565	CD	LYS	579	15.725	40.942	45.986	1.00	61.28
	2566	CE	LYS	579	14.910	41.704	47.020	1.00	61.64
	2567	NZ	LYS	579	13.708	40.953	47.492	1.00	62.20
45	2568	C	LYS	579	20.372	42.613	47.252	1.00	60.67
	2569	O	LYS	579	20.251	43.683	47.835	1.00	59.96
	2570	N	ALA	580	21.322	41.738	47.564	1.00	59.98
50	2571	CA	ALA	580	22.288	42.011	48.630	1.00	60.27
	2572	CB	ALA	580	22.721	40.713	49.304	1.00	64.73
	2573	C	ALA	580	23.505	42.722	48.059	1.00	58.96
55	2574	O	ALA	580	24.349	43.229	48.801	1.00	61.59
	2575	N	ILE	581	23.590	42.738	46.731	1.00	63.39
	2576	CA	ILE	581	24.690	43.380	46.030	1.00	60.52
60	2577	CB	ILE	581	24.789	42.908	44.559	1.00	60.74
	2578	CG2	ILE	581	25.911	43.650	43.840	1.00	63.37
	2579	CG1	ILE	581	25.069	41.409	44.494	1.00	60.26
65	2580	CD1	ILE	581	24.930	40.862	43.091	1.00	61.59

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5 2581	C	ILE	581	24.426	44.873	46.025	1.00	63.62
2582	O	ILE	581	23.418	45.329	45.482	1.00	63.59
2583	N	PRO	582	25.329	45.655	46.634	1.00	62.76
10 2584	CD	PRO	582	26.596	45.257	47.270	1.00	63.28
2585	CA	PRO	582	25.162	47.104	46.681	1.00	64.52
2586	CB	PRO	582	26.505	47.589	47.226	1.00	62.45
2587	CG	PRO	582	26.934	46.473	48.106	1.00	59.21
15 2588	C	PRO	582	24.882	47.654	45.298	1.00	62.22
2589	O	PRO	582	25.518	47.252	44.323	1.00	61.69
2590	N	GLY	583	23.913	48.560	45.224	1.00	58.26
2591	CA	GLY	583	23.565	49.189	43.965	1.00	59.81
20 2592	C	GLY	583	22.640	48.446	43.028	1.00	61.92
2593	O	GLY	583	22.231	49.002	42.024	1.00	58.88
2594	N	PHE	584	22.302	47.201	43.327	1.00	62.92
25 2595	CA	PHE	584	21.418	46.459	42.438	1.00	61.83
2596	CB	PHE	584	21.563	44.953	42.677	1.00	62.46
2597	CG	PHE	584	20.863	44.104	41.650	1.00	57.96
30 2598	CD1	PHE	584	21.406	43.921	40.390	1.00	63.14
2599	CD2	PHE	584	19.646	43.514	41.938	1.00	62.84
2600	CE1	PHE	584	20.746	43.166	39.437	1.00	61.42
2601	CE2	PHE	584	18.980	42.759	40.991	1.00	60.47
35 2602	CZ	PHE	584	19.533	42.585	39.737	1.00	59.28
2603	C	PHE	584	19.958	46.883	42.624	1.00	60.13
2604	O	PHE	584	19.210	46.996	41.653	1.00	61.49
40 2605	N	ARG	585	19.561	47.131	43.870	1.00	60.78
2606	CA	ARG	585	18.190	47.535	44.160	1.00	63.10
2607	CB	ARG	585	17.832	47.252	45.627	1.00	59.03
2608	CG	ARG	585	17.716	45.757	45.943	1.00	57.77
45 2609	CD	ARG	585	17.222	45.476	47.365	1.00	61.69
2610	NE	ARG	585	15.825	45.858	47.587	1.00	62.10
2611	CZ	ARG	585	14.800	45.492	46.817	1.00	62.77
50 2612	NH1	ARG	585	14.996	44.724	45.744	1.00	60.63
2613	NH2	ARG	585	13.569	45.893	47.126	1.00	59.26
2614	C	ARG	585	17.952	48.996	43.843	1.00	59.85
2615	O	ARG	585	16.833	49.487	43.965	1.00	61.84
55 2616	N	ASN	586	19.003	49.689	43.424	1.00	60.92
2617	CA	ASN	586	18.871	51.094	43.090	1.00	62.56

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2618	CB	ASN	586	19.987	51.892	43.740	1.00	59.81
	2619	CG	ASN	586	20.079	51.620	45.218	1.00	62.07
	2620	OD1	ASN	586	20.714	50.651	45.641	1.00	62.28
10	2621	ND2	ASN	586	19.415	52.452	46.018	1.00	56.67
	2622	C	ASN	586	18.865	51.271	41.592	1.00	63.34
	2623	O	ASN	586	19.054	52.363	41.068	1.00	60.96
15	2624	N	LEU	587	18.648	50.163	40.907	1.00	62.25
	2625	CA	LEU	587	18.551	50.166	39.467	1.00	60.33
	2626	CB	LEU	587	19.304	48.971	38.887	1.00	63.97
20	2627	CG	LEU	587	20.823	49.075	38.847	1.00	59.84
	2628	CD1	LEU	587	21.410	47.701	38.948	1.00	62.41
	2629	CD2	LEU	587	21.262	49.748	37.572	1.00	64.48
25	2630	C	LEU	587	17.053	50.008	39.259	1.00	61.19
	2631	O	LEU	587	16.355	49.541	40.164	1.00	61.87
	2632	N	HIS	588	16.556	50.400	38.090	1.00	63.05
30	2633	CA	HIS	588	15.130	50.288	37.829	1.00	58.93
	2634	CB	HIS	588	14.797	50.621	36.371	1.00	62.93
	2635	CG	HIS	588	13.338	50.871	36.131	1.00	61.44
35	2636	CD2	HIS	588	12.679	51.990	35.745	1.00	61.68
	2637	ND1	HIS	588	12.369	49.912	36.344	1.00	59.82
	2638	CE1	HIS	588	11.178	50.431	36.101	1.00	59.25
40	2639	NE2	HIS	588	11.339	51.691	35.736	1.00	58.14
	2640	C	HIS	588	14.723	48.860	38.128	1.00	61.41
	2641	O	HIS	588	15.515	47.942	37.948	1.00	59.96
45	2642	N	LEU	589	13.492	48.686	38.598	1.00	59.88
	2643	CA	LEU	589	12.974	47.370	38.929	1.00	61.54
	2644	CB	LEU	589	11.602	47.509	39.599	1.00	60.80
50	2645	CG	LEU	589	10.980	46.337	40.367	1.00	62.36
	2646	CD1	LEU	589	10.643	45.192	39.424	1.00	59.67
	2647	CD2	LEU	589	11.934	45.887	41.449	1.00	61.30
55	2648	C	LEU	589	12.867	46.562	37.640	1.00	60.73
	2649	O	LEU	589	12.841	45.332	37.667	1.00	59.26
	2650	N	ASP	590	12.811	47.254	36.507	1.00	62.77
	2651	CA	ASP	590	12.714	46.574	35.222	1.00	59.61
	2652	CB	ASP	590	12.172	47.516	34.154	1.00	60.63
	2653	CG	ASP	590	10.676	47.476	34.060	1.00	60.64
	2654	OD1	ASP	590	10.031	47.099	35.060	1.00	66.03

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2655	OD2	ASP	590	10.140	47.830	32.989	1.00	62.74
2656	C	ASP	590	14.077	46.079	34.801	1.00	64.03
2657	O	ASP	590	14.194	45.131	34.020	1.00	61.02
2658	N	ASP	591	15.109	46.734	35.319	1.00	61.76
2659	CA	ASP	591	16.481	46.364	34.993	1.00	61.72
2660	CB	ASP	591	17.425	47.557	35.224	1.00	60.28
2661	CG	ASP	591	17.174	48.709	34.250	1.00	66.48
2662	OD1	ASP	591	16.782	48.445	33.092	1.00	56.28
2663	OD2	ASP	591	17.393	49.877	34.639	1.00	63.43
2664	C	ASP	591	16.937	45.160	35.813	1.00	60.81
2665	O	ASP	591	17.642	44.292	35.306	1.00	61.99
2666	N	GLN	592	16.515	45.120	37.075	1.00	59.60
2667	CA	GLN	592	16.852	44.035	37.981	1.00	59.54
2668	CB	GLN	592	16.145	44.209	39.327	1.00	60.92
2669	CG	GLN	592	16.268	45.571	39.962	1.00	63.19
2670	CD	GLN	592	15.991	45.536	41.460	1.00	61.96
2671	OE1	GLN	592	15.303	44.641	41.967	1.00	59.41
2672	NE2	GLN	592	16.522	46.518	42.176	1.00	61.73
2673	C	GLN	592	16.409	42.711	37.376	1.00	58.77
2674	O	GLN	592	17.034	41.668	37.606	1.00	60.09
2675	N	MET	593	15.319	42.762	36.611	1.00	61.89
2676	CA	MET	593	14.756	41.575	35.977	1.00	60.29
2677	CB	MET	593	13.257	41.746	35.768	1.00	61.65
2678	CG	MET	593	12.401	41.411	36.969	1.00	61.69
2679	SD	MET	593	10.676	41.232	36.456	1.00	62.68
2680	CE	MET	593	10.249	42.940	36.274	1.00	60.78
2681	C	MET	593	15.388	41.229	34.645	1.00	59.77
2682	O	MET	593	15.386	40.068	34.241	1.00	61.16
2683	N	THR	594	15.904	42.235	33.948	1.00	59.97
2684	CA	THR	594	16.541	42.008	32.655	1.00	61.96
2685	CB	THR	594	16.828	43.335	31.932	1.00	61.57
2686	OG1	THR	594	15.726	44.234	32.127	1.00	61.11
2687	CG2	THR	594	17.026	43.086	30.435	1.00	62.41
2688	C	THR	594	17.865	41.305	32.902	1.00	63.83
2689	O	THR	594	18.184	40.287	32.274	1.00	62.47
2690	N	LEU	595	18.634	41.865	33.829	1.00	61.96
2691	CA	LEU	595	19.924	41.308	34.184	1.00	62.86

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2692	CB	LEU	595	20.585	42.172	35.265	1.00	61.42
	2693	CG	LEU	595	20.937	43.615	34.885	1.00	63.11
	2694	CD1	LEU	595	21.680	44.276	36.031	1.00	63.10
10	2695	CD2	LEU	595	21.791	43.634	33.636	1.00	59.45
	2696	C	LEU	595	19.784	39.859	34.660	1.00	61.56
	2697	O	LEU	595	20.438	38.960	34.136	1.00	62.15
15	2698	N	LEU	596	18.920	39.629	35.640	1.00	63.33
	2699	CA	LEU	596	18.728	38.283	36.156	1.00	61.25
	2700	CB	LEU	596	17.830	38.313	37.387	1.00	59.50
20	2701	CG	LEU	596	18.518	38.469	38.735	1.00	63.65
	2702	CD1	LEU	596	17.484	38.837	39.769	1.00	60.39
	2703	CD2	LEU	596	19.232	37.190	39.109	1.00	62.18
25	2704	C	LEU	596	18.159	37.293	35.140	1.00	57.46
	2705	O	LEU	596	18.306	36.079	35.310	1.00	60.98
	2706	N	GLN	597	17.507	37.800	34.095	1.00	60.24
30	2707	CA	GLN	597	16.915	36.953	33.055	1.00	59.39
	2708	CB	GLN	597	15.727	37.660	32.413	1.00	63.86
	2709	CG	GLN	597	14.431	37.528	33.171	1.00	63.29
35	2710	CD	GLN	597	13.365	38.466	32.648	1.00	58.84
	2711	OE1	GLN	597	13.389	38.873	31.484	1.00	61.11
	2712	NE2	GLN	597	12.414	38.811	33.505	1.00	60.83
40	2713	C	GLN	597	17.927	36.620	31.973	1.00	60.76
	2714	O	GLN	597	17.829	35.597	31.302	1.00	63.58
	2715	N	TYR	598	18.900	37.501	31.806	1.00	59.20
45	2716	CA	TYR	598	19.923	37.315	30.807	1.00	61.48
	2717	CB	TYR	598	20.378	38.678	30.311	1.00	64.95
	2718	CG	TYR	598	19.364	39.407	29.466	1.00	59.33
50	2719	CD1	TYR	598	18.119	38.844	29.177	1.00	59.16
	2720	CE1	TYR	598	17.213	39.496	28.344	1.00	62.34
	2721	CD2	TYR	598	19.673	40.645	28.903	1.00	58.48
55	2722	CE2	TYR	598	18.771	41.303	28.067	1.00	61.12
	2723	CZ	TYR	598	17.551	40.721	27.794	1.00	63.18
	2724	OH	TYR	598	16.680	41.371	26.960	1.00	63.83
55	2725	C	TYR	598	21.130	36.532	31.320	1.00	63.31
	2726	O	TYR	598	21.850	35.900	30.550	1.00	62.59
	2727	N	SER	599	21.356	36.554	32.623	1.00	62.16
	2728	CA	SER	599	22.511	35.859	33.157	1.00	62.80

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	2729	CB	SER	599	23.420	36.885	33.845	1.00	60.71
	2730	OG	SER	599	22.660	37.845	34.560	1.00	60.75
	2731	C	SER	599	22.245	34.678	34.093	1.00	60.81
10	2732	O	SER	599	23.183	34.104	34.636	1.00	57.53
	2733	N	TRP	600	20.986	34.293	34.272	1.00	62.86
	2734	CA	TRP	600	20.683	33.187	35.180	1.00	60.85
15	2735	CB	TRP	600	19.186	32.813	35.134	1.00	60.84
	2736	CG	TRP	600	18.745	32.104	33.887	1.00	61.86
	2737	CD2	TRP	600	18.561	30.697	33.726	1.00	61.60
20	2738	CE2	TRP	600	18.300	30.461	32.362	1.00	64.40
	2739	CE3	TRP	600	18.599	29.611	34.602	1.00	59.75
	2740	CD1	TRP	600	18.574	32.653	32.650	1.00	60.08
25	2741	NE1	TRP	600	18.311	31.672	31.724	1.00	59.13
	2742	CZ2	TRP	600	18.085	29.182	31.854	1.00	61.82
	2743	CZ3	TRP	600	18.383	28.342	34.097	1.00	63.01
30	2744	CH2	TRP	600	18.131	28.137	32.737	1.00	62.11
	2745	C	TRP	600	21.523	31.963	34.848	1.00	61.75
	2746	O	TRP	600	21.973	31.238	35.732	1.00	60.91
35	2747	N	MET	601	21.761	31.749	33.564	1.00	62.84
	2748	CA	MET	601	22.504	30.591	33.172	1.00	60.19
	2749	CB	MET	601	22.084	30.133	31.794	1.00	61.93
40	2750	CG	MET	601	22.616	28.786	31.496	1.00	63.07
	2751	SD	MET	601	21.595	27.427	31.465	1.00	62.35
	2752	CE	MET	601	22.357	26.773	32.529	1.00	60.74
45	2753	C	MET	601	24.008	30.766	33.243	1.00	61.35
	2754	O	MET	601	24.732	29.790	33.391	1.00	62.01
	2755	N	SER	602	24.483	32.002	33.146	1.00	59.64
50	2756	CA	SER	602	25.914	32.253	33.227	1.00	61.85
	2757	CB	SER	602	26.249	33.637	32.675	1.00	63.12
	2758	OG	SER	602	27.643	33.887	32.746	1.00	63.90
55	2759	C	SER	602	26.356	32.163	34.684	1.00	63.19
	2760	O	SER	602	27.478	31.765	34.976	1.00	59.89
	2761	N	LEU	603	25.452	32.537	35.588	1.00	59.89
55	2762	CA	LEU	603	25.703	32.527	37.027	1.00	63.05
	2763	CB	LEU	603	24.673	33.413	37.748	1.00	60.06
	2764	CG	LEU	603	24.752	34.936	37.606	1.00	58.80
	2765	CD1	LEU	603	23.591	35.588	38.334	1.00	59.17

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2766	CD2	LEU	603	26.051	35.422	38.175	1.00	63.89
	2767	C	LEU	603	25.624	31.118	37.586	1.00	60.06
	2768	O	LEU	603	26.337	30.753	38.519	1.00	58.30
10	2769	N	MET	604	24.745	30.323	37.004	1.00	62.50
	2770	CA	MET	604	24.565	28.967	37.468	1.00	61.20
	2771	CB	MET	604	23.151	28.541	37.166	1.00	59.34
15	2772	CG	MET	604	22.185	28.879	38.247	1.00	61.83
	2773	SD	MET	604	22.610	30.141	39.388	1.00	62.09
	2774	CE	MET	604	22.173	29.285	40.731	1.00	60.68
20	2775	C	MET	604	25.578	28.009	36.879	1.00	61.48
	2776	O	MET	604	25.989	27.048	37.536	1.00	60.91
	2777	N	ALA	605	25.988	28.292	35.646	1.00	58.39
25	2778	CA	ALA	605	26.970	27.493	34.943	1.00	62.30
	2779	CB	ALA	605	26.934	27.812	33.472	1.00	63.55
	2780	C	ALA	605	28.341	27.820	35.502	1.00	63.47
30	2781	O	ALA	605	29.194	26.944	35.590	1.00	60.63
	2782	N	PHE	606	28.546	29.082	35.882	1.00	60.75
	2783	CA	PHE	606	29.832	29.536	36.411	1.00	62.24
35	2784	CB	PHE	606	29.951	31.059	36.300	1.00	65.41
	2785	CG	PHE	606	31.316	31.606	36.663	1.00	64.45
	2786	CD1	PHE	606	32.424	31.375	35.848	1.00	62.88
40	2787	CD2	PHE	606	31.483	32.388	37.802	1.00	61.45
	2788	CE1	PHE	606	33.668	31.919	36.162	1.00	61.89
	2789	CE2	PHE	606	32.725	32.931	38.120	1.00	63.04
45	2790	CZ	PHE	606	33.814	32.696	37.296	1.00	66.17
	2791	C	PHE	606	30.044	29.121	37.851	1.00	64.34
	2792	O	PHE	606	31.154	28.764	38.234	1.00	61.04
50	2793	N	ALA	607	28.997	29.180	38.661	1.00	59.38
	2794	CA	ALA	607	29.144	28.771	40.047	1.00	61.90
	2795	CB	ALA	607	27.953	29.224	40.865	1.00	58.55
55	2796	C	ALA	607	29.269	27.246	40.073	1.00	58.23
	2797	O	ALA	607	29.912	26.681	40.953	1.00	60.68
	2798	N	LEU	608	28.656	26.571	39.110	1.00	61.24
	2799	CA	LEU	608	28.771	25.121	39.086	1.00	60.02
	2800	CB	LEU	608	27.928	24.526	37.958	1.00	62.86
	2801	CG	LEU	608	27.703	23.018	37.693	1.00	60.90
	2802	CD1	LEU	608	27.926	22.923	36.222	1.00	62.46

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2803	CD2	LEU	608	28.630	22.033	38.439	1.00	60.02
2804	C	LEU	608	30.240	24.783	38.858	1.00	61.60
2805	O	LEU	608	30.758	23.870	39.479	1.00	62.78
2806	N	GLY	609	30.917	25.511	37.974	1.00	63.89
2807	CA	GLY	609	32.319	25.229	37.746	1.00	60.11
2808	C	GLY	609	33.143	25.391	39.018	1.00	61.05
2809	O	GLY	609	34.080	24.631	39.266	1.00	62.95
2810	N	TRP	610	32.783	26.374	39.838	1.00	62.51
2811	CA	TRP	610	33.499	26.652	41.073	1.00	63.33
2812	CB	TRP	610	32.917	27.885	41.741	1.00	59.08
2813	CG	TRP	610	33.617	28.226	43.008	1.00	60.29
2814	CD2	TRP	610	34.910	28.821	43.127	1.00	61.56
2815	CE2	TRP	610	35.194	28.930	44.501	1.00	59.81
2816	CE3	TRP	610	35.860	29.273	42.200	1.00	57.77
2817	CD1	TRP	610	33.178	28.002	44.279	1.00	61.04
2818	NE1	TRP	610	34.121	28.423	45.183	1.00	63.24
2819	CZ2	TRP	610	36.387	29.472	44.973	1.00	58.16
2820	CZ3	TRP	610	37.048	29.811	42.670	1.00	62.09
2821	CH2	TRP	610	37.301	29.905	44.043	1.00	63.07
2822	C	TRP	610	33.516	25.510	42.073	1.00	62.56
2823	O	TRP	610	34.554	25.205	42.662	1.00	62.85
2824	N	ARG	611	32.360	24.896	42.288	1.00	64.01
2825	CA	ARG	611	32.268	23.784	43.222	1.00	61.00
2826	CB	ARG	611	30.803	23.396	43.440	1.00	60.82
2827	CG	ARG	611	29.973	24.437	44.180	1.00	60.63
2828	CD	ARG	611	28.568	23.899	44.480	1.00	63.65
2829	NE	ARG	611	27.830	23.608	43.250	1.00	60.05
2830	CZ	ARG	611	27.228	24.528	42.498	1.00	61.48
2831	NH1	ARG	611	27.255	25.811	42.853	1.00	62.30
2832	NH2	ARG	611	26.638	24.175	41.365	1.00	62.30
2833	C	ARG	611	33.049	22.606	42.648	1.00	64.56
2834	O	ARG	611	33.712	21.854	43.373	1.00	59.80
2835	N	SER	612	32.971	22.467	41.329	1.00	60.03
2836	CA	SER	612	33.664	21.403	40.624	1.00	62.69
2837	CB	SER	612	33.312	21.451	39.141	1.00	60.54
2838	OG	SER	612	31.976	21.038	38.947	1.00	61.90
2839	C	SER	612	35.163	21.542	40.815	1.00	60.18

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2840	O	SER	612	35.842	20.597	41.209	1.00	62.35
	2841	N	TYR	613	35.663	22.738	40.538	1.00	59.25
	2842	CA	TYR	613	37.074	23.058	40.677	1.00	60.56
10	2843	CB	TYR	613	37.265	24.534	40.311	1.00	63.42
	2844	CG	TYR	613	38.515	25.215	40.829	1.00	66.04
	2845	CD1	TYR	613	39.771	24.631	40.692	1.00	61.54
15	2846	CE1	TYR	613	40.925	25.308	41.091	1.00	59.89
	2847	CD2	TYR	613	38.443	26.491	41.384	1.00	61.40
	2848	CE2	TYR	613	39.586	27.172	41.782	1.00	60.60
20	2849	CZ	TYR	613	40.823	26.577	41.633	1.00	61.69
	2850	OH	TYR	613	41.950	27.258	42.022	1.00	57.50
	2851	C	TYR	613	37.624	22.765	42.074	1.00	61.96
25	2852	O	TYR	613	38.665	22.130	42.219	1.00	62.16
	2853	N	ARG	614	36.913	23.204	43.102	1.00	65.05
	2854	CA	ARG	614	37.380	23.004	44.463	1.00	59.34
30	2855	CB	ARG	614	36.724	24.017	45.395	1.00	60.68
	2856	CG	ARG	614	36.950	25.445	45.007	1.00	63.19
	2857	CD	ARG	614	36.724	26.354	46.190	1.00	59.94
35	2858	NE	ARG	614	37.945	26.927	46.773	1.00	59.42
	2859	CZ	ARG	614	39.115	27.068	46.145	1.00	60.26
	2860	NH1	ARG	614	40.141	27.628	46.776	1.00	60.62
40	2861	NH2	ARG	614	39.288	26.619	44.906	1.00	59.69
	2862	C	ARG	614	37.144	21.620	45.019	1.00	60.75
	2863	O	ARG	614	37.899	21.144	45.869	1.00	61.95
45	2864	N	GLN	615	36.093	20.967	44.549	1.00	60.97
	2865	CA	GLN	615	35.780	19.654	45.074	1.00	61.36
	2866	CB	GLN	615	34.282	19.387	44.957	1.00	59.74
50	2867	CG	GLN	615	33.666	18.942	46.273	1.00	65.30
	2868	CD	GLN	615	32.416	18.106	46.097	1.00	64.80
	2869	OE1	GLN	615	32.019	17.380	47.007	1.00	59.65
55	2870	NE2	GLN	615	31.787	18.204	44.928	1.00	63.88
	2871	C	GLN	615	36.547	18.523	44.419	1.00	61.87
	2872	O	GLN	615	36.984	17.588	45.093	1.00	61.19
55	2873	N	SER	616	36.726	18.615	43.109	1.00	62.69
	2874	CA	SER	616	37.408	17.559	42.387	1.00	60.64
	2875	CB	SER	616	36.380	16.632	41.757	1.00	64.46
	2876	OG	SER	616	35.731	17.299	40.688	1.00	63.47

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	2877	C	SER	616	38.347	18.047	41.298	1.00	59.36
	2878	O	SER	616	38.444	17.424	40.246	1.00	61.79
	2879	N	SER	617	39.021	19.163	41.534	1.00	62.74
10	2880	CA	SER	617	39.972	19.681	40.560	1.00	60.01
	2881	CB	SER	617	41.253	18.847	40.638	1.00	56.86
	2882	OG	SER	617	41.690	18.714	41.980	1.00	64.58
15	2883	C	SER	617	39.433	19.675	39.119	1.00	62.31
	2884	O	SER	617	40.099	19.196	38.196	1.00	60.08
	2885	N	ALA	618	38.230	20.213	38.931	1.00	62.60
20	2886	CA	ALA	618	37.600	20.261	37.612	1.00	62.84
	2887	CB	ALA	618	38.399	21.165	36.676	1.00	61.64
	2888	C	ALA	618	37.475	18.866	37.005	1.00	60.94
25	2889	O	ALA	618	37.175	18.725	35.820	1.00	63.12
	2890	N	ASN	619	37.692	17.836	37.820	1.00	60.02
	2891	CA	ASN	619	37.610	16.465	37.330	1.00	60.02
30	2892	CB	ASN	619	38.467	15.523	38.178	1.00	61.65
	2893	CG	ASN	619	39.881	15.426	37.663	1.00	65.19
	2894	OD1	ASN	619	40.813	15.986	38.241	1.00	58.62
35	2895	ND2	ASN	619	40.047	14.729	36.547	1.00	59.93
	2896	C	ASN	619	36.205	15.922	37.241	1.00	63.97
	2897	O	ASN	619	35.933	15.005	36.469	1.00	61.24
40	2898	N	LEU	620	35.305	16.487	38.028	1.00	61.46
	2899	CA	LEU	620	33.925	16.044	37.999	1.00	61.85
	2900	CB	LEU	620	33.599	15.266	39.271	1.00	63.36
45	2901	CG	LEU	620	34.516	14.087	39.589	1.00	60.08
	2902	CD1	LEU	620	33.992	13.354	40.805	1.00	65.17
	2903	CD2	LEU	620	34.578	13.145	38.408	1.00	59.21
50	2904	C	LEU	620	33.031	17.266	37.890	1.00	63.79
	2905	O	LEU	620	33.520	18.400	37.844	1.00	62.56
	2906	N	LEU	621	31.728	17.022	37.808	1.00	60.88
55	2907	CA	LEU	621	30.757	18.096	37.739	1.00	60.93
	2908	CB	LEU	621	29.822	17.930	36.545	1.00	59.84
	2909	CG	LEU	621	30.365	18.564	35.272	1.00	61.52
	2910	CD1	LEU	621	29.302	18.516	34.204	1.00	61.79
	2911	CD2	LEU	621	30.776	19.998	35.547	1.00	62.82
	2912	C	LEU	621	30.001	17.973	39.033	1.00	59.84
	2913	O	LEU	621	29.267	17.009	39.249	1.00	59.39

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2914	N	CYS	622	30.191	18.952	39.903	1.00	60.82
	2915	CA	CYS	622	29.562	18.902	41.201	1.00	61.70
	2916	CB	CYS	622	30.612	19.216	42.276	1.00	61.70
10	2917	SG	CYS	622	32.249	18.417	42.005	1.00	55.72
	2918	C	CYS	622	28.360	19.822	41.333	1.00	60.92
	2919	O	CYS	622	28.394	20.777	42.107	1.00	60.85
15	2920	N	PHE	623	27.299	19.518	40.584	1.00	62.83
	2921	CA	PHE	623	26.057	20.298	40.618	1.00	61.52
	2922	CB	PHE	623	24.944	19.578	39.827	1.00	63.16
20	2923	CG	PHE	623	25.174	19.562	38.332	1.00	64.30
	2924	CD1	PHE	623	25.946	18.565	37.734	1.00	62.97
	2925	CD2	PHE	623	24.667	20.580	37.527	1.00	59.44
25	2926	CE1	PHE	623	26.214	18.585	36.354	1.00	60.51
	2927	CE2	PHE	623	24.931	20.607	36.152	1.00	61.00
	2928	CZ	PHE	623	25.705	19.609	35.566	1.00	58.20
30	2929	C	PHE	623	25.631	20.512	42.074	1.00	62.99
	2930	O	PHE	623	25.433	21.650	42.520	1.00	59.63
	2931	N	ALA	624	25.489	19.404	42.798	1.00	60.19
35	2932	CA	ALA	624	25.146	19.426	44.220	1.00	60.71
	2933	CB	ALA	624	23.953	18.540	44.505	1.00	65.97
	2934	C	ALA	624	26.384	18.877	44.921	1.00	60.87
40	2935	O	ALA	624	27.278	18.328	44.276	1.00	61.88
	2936	N	PRO	625	26.467	19.023	46.248	1.00	63.71
	2937	CD	PRO	625	25.561	19.666	47.207	1.00	59.14
45	2938	CA	PRO	625	27.658	18.496	46.924	1.00	61.58
	2939	CB	PRO	625	27.528	19.055	48.346	1.00	64.33
	2940	CG	PRO	625	26.534	20.184	48.212	1.00	61.92
50	2941	C	PRO	625	27.593	16.960	46.904	1.00	61.41
	2942	O	PRO	625	28.630	16.280	46.869	1.00	60.49
	2943	N	ASP	626	26.353	16.450	46.913	1.00	61.38
55	2944	CA	ASP	626	26.036	15.016	46.914	1.00	61.12
	2945	CB	ASP	626	25.050	14.730	48.038	1.00	59.24
	2946	CG	ASP	626	23.643	15.219	47.706	1.00	60.93
	2947	OD1	ASP	626	23.518	16.271	47.036	1.00	62.15
	2948	OD2	ASP	626	22.658	14.564	48.112	1.00	64.40
	2949	C	ASP	626	25.405	14.562	45.587	1.00	62.42
	2950	O	ASP	626	24.526	13.703	45.568	1.00	60.54

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
2951	N	LEU	627	25.834	15.152	44.483	1.00	60.30
2952	CA	LEU	627	25.293	14.792	43.183	1.00	61.38
2953	CB	LEU	627	24.007	15.569	42.915	1.00	59.07
2954	CG	LEU	627	23.311	15.347	41.573	1.00	62.30
2955	CD1	LEU	627	22.632	13.994	41.525	1.00	59.92
2956	CD2	LEU	627	22.300	16.440	41.381	1.00	64.94
2957	C	LEU	627	26.349	15.143	42.152	1.00	59.24
2958	O	LEU	627	26.321	16.224	41.550	1.00	60.06
2959	N	ILE	628	27.284	14.219	41.958	1.00	59.89
2960	CA	ILE	628	28.380	14.422	41.030	1.00	60.40
2961	CB	ILE	628	29.729	14.056	41.692	1.00	62.59
2962	CG2	ILE	628	30.850	14.267	40.716	1.00	59.44
2963	CG1	ILE	628	29.990	14.940	42.909	1.00	61.86
2964	CD1	ILE	628	29.045	14.711	44.049	1.00	62.51
2965	C	ILE	628	28.234	13.609	39.750	1.00	64.22
2966	O	ILE	628	28.028	12.402	39.787	1.00	60.75
2967	N	ILE	629	28.323	14.272	38.608	1.00	60.54
2968	CA	ILE	629	28.239	13.540	37.370	1.00	62.37
2969	CB	ILE	629	28.044	14.470	36.165	1.00	65.41
2970	CG2	ILE	629	28.371	13.733	34.877	1.00	61.37
2971	CG1	ILE	629	26.619	15.024	36.170	1.00	63.05
2972	CD1	ILE	629	25.623	14.193	36.983	1.00	60.63
2973	C	ILE	629	29.575	12.839	37.270	1.00	60.22
2974	O	ILE	629	30.580	13.454	36.929	1.00	58.35
2975	N	ASN	630	29.580	11.556	37.611	1.00	60.04
2976	CA	ASN	630	30.776	10.726	37.570	1.00	60.83
2977	CB	ASN	630	30.674	9.637	38.632	1.00	62.77
2978	CG	ASN	630	29.368	8.868	38.556	1.00	60.79
2979	OD1	ASN	630	29.051	8.248	37.541	1.00	61.32
2980	ND2	ASN	630	28.603	8.908	39.632	1.00	62.90
2981	C	ASN	630	30.949	10.085	36.197	1.00	60.61
2982	O	ASN	630	30.016	10.041	35.403	1.00	62.50
2983	N	GLU	631	32.151	9.592	35.926	1.00	63.77
2984	CA	GLU	631	32.472	8.954	34.653	1.00	60.65
2985	CB	GLU	631	33.804	8.219	34.786	1.00	62.06
2986	CG	GLU	631	34.021	7.046	33.841	1.00	63.14
2987	CD	GLU	631	35.255	6.229	34.232	1.00	59.80

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	2988	OE1	GLU	631	36.349	6.836	34.405	1.00	61.43
	2989	OE2	GLU	631	35.122	4.988	34.369	1.00	58.68
	2990	C	GLU	631	31.381	7.986	34.254	1.00	61.07
10	2991	O	GLU	631	30.879	8.014	33.132	1.00	61.02
	2992	N	GLN	632	31.011	7.126	35.186	1.00	63.77
	2993	CA	GLN	632	29.978	6.151	34.916	1.00	61.66
15	2994	CB	GLN	632	29.732	5.285	36.159	1.00	61.41
	2995	CG	GLN	632	30.936	4.415	36.579	1.00	65.26
	2996	CD	GLN	632	31.704	3.828	35.393	1.00	64.37
20	2997	OE1	GLN	632	31.109	3.357	34.420	1.00	60.73
	2998	NE2	GLN	632	33.034	3.847	35.480	1.00	59.46
	2999	C	GLN	632	28.695	6.851	34.466	1.00	61.12
25	3000	O	GLN	632	28.055	6.417	33.512	1.00	62.13
	3001	N	ARG	633	28.334	7.946	35.134	1.00	59.27
	3002	CA	ARG	633	27.125	8.682	34.767	1.00	61.29
30	3003	CB	ARG	633	26.821	9.786	35.775	1.00	59.65
	3004	CG	ARG	633	26.235	9.274	37.069	1.00	62.42
	3005	CD	ARG	633	25.223	10.258	37.602	1.00	60.12
35	3006	NE	ARG	633	24.486	9.732	38.743	1.00	61.79
	3007	CZ	ARG	633	24.739	10.038	40.011	1.00	64.89
	3008	NH1	ARG	633	25.717	10.878	40.308	1.00	60.64
40	3009	NH2	ARG	633	24.014	9.501	40.984	1.00	62.92
	3010	C	ARG	633	27.151	9.274	33.360	1.00	61.86
	3011	O	ARG	633	26.086	9.401	32.750	1.00	59.63
45	3012	N	MET	634	28.337	9.643	32.855	1.00	64.70
	3013	CA	MET	634	28.465	10.180	31.497	1.00	60.91
	3014	CB	MET	634	29.921	10.556	31.189	1.00	59.90
50	3015	CG	MET	634	30.438	11.791	31.950	1.00	60.63
	3016	SD	MET	634	30.042	13.425	31.192	1.00	60.35
	3017	CE	MET	634	30.985	14.531	32.251	1.00	64.03
55	3018	C	MET	634	27.956	9.086	30.543	1.00	60.81
	3019	O	MET	634	28.727	8.350	29.899	1.00	62.71
	3020	N	THR	635	26.622	8.989	30.531	1.00	62.02
	3021	CA	THR	635	25.820	8.059	29.738	1.00	62.69
	3022	CB	THR	635	24.313	8.140	30.124	1.00	62.75
	3023	OG1	THR	635	24.150	7.893	31.528	1.00	60.63
	3024	CG2	THR	635	23.486	7.141	29.303	1.00	61.43

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	3025	C	THR	635	25.912	8.531	28.307	1.00	61.30
	3026	O	THR	635	26.510	7.876	27.454	1.00	59.84
	3027	N	LEU	636	25.315	9.694	28.077	1.00	61.92
10	3028	CA	LEU	636	25.270	10.317	26.765	1.00	60.40
	3029	CB	LEU	636	23.901	10.968	26.586	1.00	63.75
	3030	CG	LEU	636	22.679	10.156	26.167	1.00	61.04
15	3031	CD1	LEU	636	22.623	8.760	26.811	1.00	59.92
	3032	CD2	LEU	636	21.476	11.011	26.536	1.00	55.92
	3033	C	LEU	636	26.347	11.377	26.441	1.00	63.57
20	3034	O	LEU	636	26.834	12.087	27.327	1.00	58.28
	3035	N	PRO	637	26.754	11.471	25.155	1.00	61.79
	3036	CD	PRO	637	26.479	10.631	23.987	1.00	63.46
25	3037	CA	PRO	637	27.744	12.476	24.794	1.00	60.89
	3038	CB	PRO	637	28.363	11.932	23.490	1.00	63.07
	3039	CG	PRO	637	27.855	10.482	23.398	1.00	62.95
30	3040	C	PRO	637	26.780	13.647	24.551	1.00	61.80
	3041	O	PRO	637	27.038	14.531	23.736	1.00	60.33
	3042	N	CYS	638	25.605	13.523	25.193	1.00	63.35
35	3043	CA	CYS	638	24.557	14.549	25.225	1.00	58.89
	3044	CB	CYS	638	23.122	14.023	25.351	1.00	62.48
	3045	SG	CYS	638	22.633	12.668	24.333	1.00	61.93
40	3046	C	CYS	638	24.925	14.896	26.642	1.00	59.34
	3047	O	CYS	638	25.366	16.010	26.968	1.00	61.64
	3048	N	MET	639	24.773	13.878	27.486	1.00	59.95
45	3049	CA	MET	639	25.094	14.058	28.870	1.00	62.51
	3050	CB	MET	639	24.794	12.794	29.647	1.00	56.25
	3051	CG	MET	639	24.597	13.021	31.126	1.00	59.11
50	3052	SD	MET	639	23.446	14.225	31.808	1.00	60.73
	3053	CE	MET	639	24.286	14.281	33.307	1.00	59.61
	3054	C	MET	639	26.567	14.451	28.934	1.00	60.92
55	3055	O	MET	639	27.074	14.783	30.000	1.00	59.57
	3056	N	TYR	640	27.244	14.409	27.782	1.00	60.93
	3057	CA	TYR	640	28.622	14.866	27.693	1.00	62.32
	3058	CB	TYR	640	29.585	13.827	27.110	1.00	61.41
	3059	CG	TYR	640	30.961	14.446	26.910	1.00	62.45
	3060	CD1	TYR	640	31.797	14.687	28.006	1.00	59.75
	3061	CE1	TYR	640	32.996	15.372	27.862	1.00	59.57

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3062	CD2	TYR	640	31.376	14.906	25.651	1.00	59.20
	3063	CE2	TYR	640	32.578	15.594	25.495	1.00	64.39
	3064	CZ	TYR	640	33.381	15.827	26.608	1.00	62.16
10	3065	OH	TYR	640	34.554	16.542	26.485	1.00	62.68
	3066	C	TYR	640	28.650	16.082	26.764	1.00	60.42
	3067	O	TYR	640	29.264	17.104	27.075	1.00	62.43
15	3068	N	ASP	641	27.985	15.960	25.619	1.00	63.11
	3069	CA	ASP	641	27.946	17.029	24.617	1.00	64.46
	3070	CB	ASP	641	26.821	16.780	23.617	1.00	64.30
20	3071	CG	ASP	641	27.232	17.039	22.196	1.00	61.31
	3072	OD1	ASP	641	26.317	17.192	21.353	1.00	59.56
	3073	OD2	ASP	641	28.453	17.079	21.917	1.00	63.20
25	3074	C	ASP	641	27.729	18.401	25.222	1.00	61.02
	3075	O	ASP	641	28.073	19.417	24.617	1.00	60.07
	3076	N	GLN	642	27.124	18.417	26.406	1.00	63.30
30	3077	CA	GLN	642	26.801	19.653	27.115	1.00	60.83
	3078	CB	GLN	642	25.298	19.837	27.180	1.00	63.77
	3079	CG	GLN	642	24.570	18.590	26.781	1.00	59.93
35	3080	CD	GLN	642	24.905	18.192	25.345	1.00	61.47
	3081	OE1	GLN	642	24.656	17.063	24.922	1.00	59.50
	3082	NE2	GLN	642	25.462	19.135	24.580	1.00	60.78
40	3083	C	GLN	642	27.353	19.664	28.518	1.00	60.90
	3084	O	GLN	642	27.430	20.714	29.136	1.00	60.17
	3085	N	CYS	643	27.678	18.497	29.052	1.00	61.78
45	3086	CA	CYS	643	28.291	18.491	30.362	1.00	62.44
	3087	CB	CYS	643	28.348	17.080	30.963	1.00	66.84
	3088	SG	CYS	643	27.004	16.704	32.130	1.00	64.90
50	3089	C	CYS	643	29.691	18.976	30.015	1.00	61.39
	3090	O	CYS	643	30.377	19.587	30.836	1.00	61.37
	3091	N	LYS	644	30.093	18.726	28.768	1.00	63.75
55	3092	CA	LYS	644	31.415	19.128	28.308	1.00	59.22
	3093	CB	LYS	644	31.708	18.603	26.889	1.00	57.84
	3094	CG	LYS	644	31.163	19.462	25.740	1.00	63.56
55	3095	CD	LYS	644	31.637	18.994	24.350	1.00	63.09
	3096	CE	LYS	644	33.034	19.520	23.983	1.00	63.23
	3097	NZ	LYS	644	34.141	19.025	24.872	1.00	61.68
	3098	C	LYS	644	31.560	20.641	28.319	1.00	61.63

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
3099	O	LYS	644	32.672	21.157	28.379	1.00	62.21
3100	N	HIS	645	30.444	21.359	28.267	1.00	59.46
3101	CA	HIS	645	30.518	22.809	28.261	1.00	61.40
3102	CB	HIS	645	29.338	23.380	27.490	1.00	62.01
3103	CG	HIS	645	29.548	23.365	26.009	1.00	61.11
3104	CD2	HIS	645	30.591	23.797	25.261	1.00	62.23
3105	ND1	HIS	645	28.628	22.845	25.123	1.00	62.89
3106	CE1	HIS	645	29.097	22.957	23.892	1.00	60.35
3107	NE2	HIS	645	30.285	23.532	23.948	1.00	58.72
3108	C	HIS	645	30.626	23.413	29.652	1.00	60.22
3109	O	HIS	645	31.097	24.535	29.804	1.00	62.73
3110	N	MET	646	30.205	22.672	30.668	1.00	61.99
3111	CA	MET	646	30.320	23.173	32.027	1.00	60.02
3112	CB	MET	646	29.235	22.574	32.963	1.00	60.39
3113	CG	MET	646	27.846	22.502	32.348	1.00	59.13
3114	SD	MET	646	26.508	21.807	33.298	1.00	59.17
3115	CE	MET	646	25.617	21.251	31.946	1.00	56.97
3116	C	MET	646	31.712	22.761	32.539	1.00	61.22
3117	O	MET	646	32.329	23.495	33.304	1.00	59.33
3118	N	LEU	647	32.207	21.597	32.110	1.00	61.22
3119	CA	LEU	647	33.539	21.146	32.526	1.00	59.88
3120	CB	LEU	647	33.858	19.754	31.962	1.00	64.23
3121	CG	LEU	647	33.205	18.494	32.529	1.00	60.79
3122	CD1	LEU	647	33.267	17.423	31.475	1.00	61.72
3123	CD2	LEU	647	33.901	18.030	33.803	1.00	62.44
3124	C	LEU	647	34.571	22.141	31.997	1.00	62.52
3125	O	LEU	647	35.664	22.292	32.558	1.00	59.55
3126	N	TYR	648	34.220	22.816	30.907	1.00	61.57
3127	CA	TYR	648	35.126	23.785	30.320	1.00	63.01
3128	CB	TYR	648	34.597	24.318	28.997	1.00	64.69
3129	CG	TYR	648	35.477	25.427	28.499	1.00	60.08
3130	CD1	TYR	648	36.741	25.148	27.989	1.00	62.71
3131	CE1	TYR	648	37.617	26.170	27.642	1.00	56.16
3132	CD2	TYR	648	35.104	26.764	28.646	1.00	65.58
3133	CE2	TYR	648	35.974	27.795	28.305	1.00	64.32
3134	CZ	TYR	648	37.226	27.490	27.806	1.00	62.44
3135	OH	TYR	648	38.097	28.500	27.480	1.00	58.63

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3136	C	TYR	648	35.380	24.969	31.241	1.00	60.50
	3137	O	TYR	648	36.510	25.423	31.369	1.00	59.77
	3138	N	VAL	649	34.331	25.490	31.865	1.00	61.19
10	3139	CA	VAL	649	34.521	26.625	32.754	1.00	62.10
	3140	CB	VAL	649	33.164	27.231	33.257	1.00	63.18
	3141	CG1	VAL	649	32.254	27.546	32.089	1.00	60.09
15	3142	CG2	VAL	649	32.476	26.282	34.202	1.00	59.25
	3143	C	VAL	649	35.313	26.111	33.941	1.00	63.47
	3144	O	VAL	649	36.188	26.791	34.465	1.00	58.78
20	3145	N	SER	650	35.010	24.884	34.340	1.00	61.57
	3146	CA	SER	650	35.664	24.258	35.471	1.00	62.45
	3147	CB	SER	650	35.032	22.901	35.727	1.00	63.87
25	3148	OG	SER	650	35.312	22.468	37.037	1.00	57.30
	3149	C	SER	650	37.152	24.102	35.217	1.00	61.59
	3150	O	SER	650	37.966	24.254	36.123	1.00	59.77
30	3151	N	SER	651	37.506	23.796	33.977	1.00	61.81
	3152	CA	SER	651	38.904	23.629	33.615	1.00	59.44
	3153	CB	SER	651	39.029	23.147	32.175	1.00	61.10
35	3154	OG	SER	651	40.285	23.527	31.635	1.00	62.25
	3155	C	SER	651	39.638	24.942	33.755	1.00	62.21
	3156	O	SER	651	40.736	24.994	34.299	1.00	59.39
40	3157	N	GLU	652	39.019	25.998	33.248	1.00	60.68
	3158	CA	GLU	652	39.590	27.333	33.296	1.00	62.47
	3159	CB	GLU	652	38.683	28.294	32.534	1.00	62.00
45	3160	CG	GLU	652	38.551	27.905	31.087	1.00	60.93
	3161	CD	GLU	652	39.896	27.841	30.412	1.00	62.60
	3162	OE1	GLU	652	40.389	28.912	29.994	1.00	61.37
50	3163	OE2	GLU	652	40.466	26.727	30.323	1.00	62.86
	3164	C	GLU	652	39.803	27.829	34.719	1.00	59.21
	3165	O	GLU	652	40.843	28.404	35.040	1.00	60.26
55	3166	N	LEU	653	38.812	27.613	35.573	1.00	62.17
	3167	CA	LEU	653	38.939	28.039	36.949	1.00	61.29
	3168	CB	LEU	653	37.630	27.816	37.702	1.00	62.27
55	3169	CG	LEU	653	36.539	28.833	37.355	1.00	63.87
	3170	CD1	LEU	653	35.239	28.428	38.009	1.00	60.88
	3171	CD2	LEU	653	36.969	30.220	37.805	1.00	66.93
	3172	C	LEU	653	40.065	27.252	37.579	1.00	61.64

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
3173	O	LEU	653	40.705	27.711	38.526	1.00	62.53
3174	N	HIS	654	40.316	26.067	37.035	1.00	59.14
3175	CA	HIS	654	41.386	25.219	37.534	1.00	63.27
3176	CB	HIS	654	41.122	23.768	37.166	1.00	63.36
3177	CG	HIS	654	42.203	22.842	37.610	1.00	63.44
3178	CD2	HIS	654	43.298	22.379	36.965	1.00	60.81
3179	ND1	HIS	654	42.281	22.360	38.898	1.00	62.60
3180	CE1	HIS	654	43.382	21.642	39.027	1.00	56.60
3181	NE2	HIS	654	44.017	21.639	37.870	1.00	63.72
3182	C	HIS	654	42.719	25.654	36.928	1.00	61.86
3183	O	HIS	654	43.691	25.906	37.636	1.00	63.73
3184	N	ARG	655	42.744	25.732	35.605	1.00	62.82
3185	CA	ARG	655	43.929	26.133	34.867	1.00	60.68
3186	CB	ARG	655	43.559	26.326	33.394	1.00	56.53
3187	CG	ARG	655	44.577	27.074	32.574	1.00	62.54
3188	CD	ARG	655	43.921	27.870	31.451	1.00	58.99
3189	NE	ARG	655	44.865	28.859	30.951	1.00	62.01
3190	CZ	ARG	655	46.081	28.544	30.503	1.00	59.65
3191	NH1	ARG	655	46.475	27.269	30.488	1.00	58.86
3192	NH2	ARG	655	46.926	29.491	30.103	1.00	59.91
3193	C	ARG	655	44.525	27.419	35.430	1.00	59.56
3194	O	ARG	655	45.741	27.524	35.595	1.00	60.27
3195	N	LEU	656	43.664	28.389	35.735	1.00	64.27
3196	CA	LEU	656	44.102	29.687	36.250	1.00	58.78
3197	CB	LEU	656	43.099	30.751	35.833	1.00	62.45
3198	CG	LEU	656	43.072	30.957	34.328	1.00	57.52
3199	CD1	LEU	656	41.832	31.704	33.943	1.00	65.67
3200	CD2	LEU	656	44.305	31.714	33.895	1.00	62.85
3201	C	LEU	656	44.340	29.761	37.757	1.00	61.09
3202	O	LEU	656	44.995	30.688	38.244	1.00	62.48
3203	N	GLN	657	43.816	28.783	38.489	1.00	59.08
3204	CA	GLN	657	43.979	28.736	39.936	1.00	63.09
3205	CB	GLN	657	45.469	28.663	40.307	1.00	58.16
3206	CG	GLN	657	46.052	27.250	40.286	1.00	63.46
3207	CD	GLN	657	45.307	26.310	41.225	1.00	59.61
3208	OE1	GLN	657	44.607	25.392	40.785	1.00	64.27
3209	NE2	GLN	657	45.442	26.547	42.529	1.00	59.12

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3210	C	GLN	657	43.335	29.932	40.611	1.00	59.19
	3211	O	GLN	657	43.926	30.539	41.498	1.00	61.22
	3212	N	VAL	658	42.113	30.249	40.192	1.00	61.76
10	3213	CA	VAL	658	41.355	31.376	40.734	1.00	61.31
	3214	CB	VAL	658	39.970	31.503	40.043	1.00	60.50
	3215	CG1	VAL	658	39.211	32.664	40.623	1.00	59.45
15	3216	CG2	VAL	658	40.132	31.716	38.559	1.00	61.37
	3217	C	VAL	658	41.115	31.283	42.240	1.00	58.30
	3218	O	VAL	658	40.838	30.208	42.764	1.00	56.60
20	3219	N	SER	659	41.214	32.418	42.928	1.00	60.76
	3220	CA	SER	659	40.979	32.465	44.369	1.00	59.93
	3221	CB	SER	659	41.873	33.507	45.047	1.00	59.20
25	3222	OG	SER	659	41.582	34.817	44.608	1.00	62.34
	3223	C	SER	659	39.518	32.789	44.656	1.00	62.94
	3224	O	SER	659	38.784	33.247	43.780	1.00	58.10
30	3225	N	TYR	660	39.097	32.563	45.893	1.00	61.68
	3226	CA	TYR	660	37.720	32.808	46.250	1.00	62.54
	3227	CB	TYR	660	37.481	32.526	47.717	1.00	64.73
35	3228	CG	TYR	660	36.014	32.432	48.044	1.00	56.73
	3229	CD1	TYR	660	35.144	31.742	47.200	1.00	59.62
	3230	CE1	TYR	660	33.817	31.568	47.524	1.00	61.29
40	3231	CD2	TYR	660	35.507	32.957	49.223	1.00	64.06
	3232	CE2	TYR	660	34.176	32.789	49.557	1.00	61.23
	3233	CZ	TYR	660	33.336	32.085	48.705	1.00	60.34
45	3234	OH	TYR	660	32.032	31.840	49.064	1.00	61.17
	3235	C	TYR	660	37.250	34.204	45.954	1.00	61.20
	3236	O	TYR	660	36.162	34.383	45.433	1.00	65.37
50	3237	N	GLU	661	38.057	35.199	46.290	1.00	61.50
	3238	CA	GLU	661	37.657	36.574	46.052	1.00	58.24
	3239	CB	GLU	661	38.598	37.523	46.765	1.00	64.85
55	3240	CG	GLU	661	38.276	37.577	48.225	1.00	61.43
	3241	CD	GLU	661	39.283	38.360	48.991	1.00	60.83
	3242	OE1	GLU	661	39.961	39.204	48.365	1.00	59.88
55	3243	OE2	GLU	661	39.387	38.143	50.219	1.00	59.48
	3244	C	GLU	661	37.548	36.918	44.591	1.00	58.50
	3245	O	GLU	661	36.573	37.536	44.178	1.00	62.37
	3246	N	GLU	662	38.529	36.516	43.798	1.00	63.69

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	3247	CA	GLU	662	38.453	36.784	42.374	1.00	59.27
	3248	CB	GLU	662	39.646	36.158	41.657	1.00	57.91
	3249	CG	GLU	662	40.974	36.663	42.122	1.00	62.43
	3250	CD	GLU	662	42.104	35.948	41.436	1.00	62.15
10	3251	OE1	GLU	662	41.969	34.732	41.223	1.00	57.52
	3252	OE2	GLU	662	43.128	36.585	41.119	1.00	61.99
	3253	C	GLU	662	37.138	36.188	41.831	1.00	61.83
15	3254	O	GLU	662	36.492	36.771	40.963	1.00	63.75
	3255	N	TYR	663	36.751	35.031	42.361	1.00	59.76
	3256	CA	TYR	663	35.525	34.336	41.962	1.00	62.22
	3257	CB	TYR	663	35.439	32.992	42.694	1.00	58.01
20	3258	CG	TYR	663	34.073	32.342	42.676	1.00	62.53
	3259	CD1	TYR	663	33.536	31.831	41.499	1.00	60.26
	3260	CE1	TYR	663	32.298	31.201	41.495	1.00	62.40
25	3261	CD2	TYR	663	33.330	32.212	43.850	1.00	58.63
	3262	CE2	TYR	663	32.096	31.590	43.855	1.00	62.25
	3263	CZ	TYR	663	31.587	31.084	42.676	1.00	63.25
30	3264	OH	TYR	663	30.372	30.448	42.682	1.00	62.04
	3265	C	TYR	663	34.240	35.125	42.228	1.00	61.08
	3266	O	TYR	663	33.429	35.343	41.322	1.00	58.41
35	3267	N	LEU	664	34.055	35.528	43.480	1.00	60.59
	3268	CA	LEU	664	32.876	36.270	43.884	1.00	61.06
	3269	CB	LEU	664	32.976	36.618	45.369	1.00	63.96
	3270	CG	LEU	664	33.063	35.440	46.343	1.00	63.81
40	3271	CD1	LEU	664	33.322	35.929	47.750	1.00	60.79
	3272	CD2	LEU	664	31.786	34.656	46.283	1.00	58.66
	3273	C	LEU	664	32.692	37.539	43.057	1.00	62.83
	3274	O	LEU	664	31.558	37.955	42.812	1.00	59.88
45	3275	N	CYS	665	33.809	38.139	42.632	1.00	59.97
	3276	CA	CYS	665	33.805	39.365	41.831	1.00	63.59
	3277	CB	CYS	665	35.167	40.043	41.869	1.00	60.16
50	3278	SG	CYS	665	35.586	40.757	43.441	1.00	62.94
	3279	C	CYS	665	33.475	39.091	40.388	1.00	60.01
	3280	O	CYS	665	32.794	39.876	39.735	1.00	57.49
55	3281	N	MET	666	33.997	37.984	39.883	1.00	60.45
	3282	CA	MET	666	33.752	37.601	38.510	1.00	61.35
	3283	CB	MET	666	34.733	36.517	38.077	1.00	60.05

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3284	CG	MET	666	36.156	36.993	37.902	1.00	63.77
	3285	SD	MET	666	37.274	35.592	37.856	1.00	59.75
	3286	CE	MET	666	37.139	35.071	36.150	1.00	62.17
10	3287	C	MET	666	32.338	37.078	38.411	1.00	61.52
	3288	O	MET	666	31.681	37.255	37.388	1.00	60.47
	3289	N	LYS	667	31.869	36.433	39.475	1.00	61.04
15	3290	CA	LYS	667	30.516	35.898	39.482	1.00	62.69
	3291	CB	LYS	667	30.261	35.036	40.726	1.00	61.46
	3292	CG	LYS	667	28.966	34.228	40.671	1.00	59.84
20	3293	CD	LYS	667	28.678	33.497	41.975	1.00	63.25
	3294	CE	LYS	667	28.483	34.471	43.123	1.00	59.23
	3295	NZ	LYS	667	27.639	33.891	44.192	1.00	61.97
25	3296	C	LYS	667	29.554	37.066	39.461	1.00	63.05
	3297	O	LYS	667	28.459	36.945	38.942	1.00	60.65
	3298	N	THR	668	29.981	38.201	40.011	1.00	61.58
30	3299	CA	THR	668	29.146	39.398	40.061	1.00	60.37
	3300	CB	THR	668	29.609	40.357	41.149	1.00	59.81
	3301	OG1	THR	668	29.776	39.634	42.370	1.00	59.26
35	3302	CG2	THR	668	28.588	41.442	41.365	1.00	57.52
	3303	C	THR	668	29.174	40.146	38.746	1.00	60.69
	3304	O	THR	668	28.184	40.749	38.348	1.00	61.79
40	3305	N	LEU	669	30.320	40.111	38.076	1.00	58.82
	3306	CA	LEU	669	30.479	40.774	36.786	1.00	60.62
	3307	CB	LEU	669	31.947	40.863	36.412	1.00	60.70
45	3308	CG	LEU	669	32.673	41.944	37.192	1.00	61.83
	3309	CD1	LEU	669	34.131	41.996	36.761	1.00	63.30
	3310	CD2	LEU	669	31.981	43.275	36.953	1.00	62.82
50	3311	C	LEU	669	29.736	40.028	35.707	1.00	63.57
	3312	O	LEU	669	29.574	40.521	34.599	1.00	63.32
	3313	N	LEU	670	29.303	38.823	36.034	1.00	62.04
55	3314	CA	LEU	670	28.558	38.030	35.087	1.00	64.79
	3315	CB	LEU	670	28.662	36.542	35.432	1.00	63.41
	3316	CG	LEU	670	29.983	35.838	35.078	1.00	62.66
	3317	CD1	LEU	670	29.918	34.407	35.554	1.00	61.38
	3318	CD2	LEU	670	30.239	35.867	33.580	1.00	61.74
	3319	C	LEU	670	27.111	38.495	35.114	1.00	60.65
	3320	O	LEU	670	26.405	38.402	34.119	1.00	60.67

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
3321	N	LEU	671	26.673	39.008	36.257	1.00	60.80
3322	CA	LEU	671	25.308	39.500	36.386	1.00	60.13
3323	CB	LEU	671	24.977	39.756	37.852	1.00	55.83
3324	CG	LEU	671	23.636	40.403	38.198	1.00	59.73
3325	CD1	LEU	671	22.495	39.498	37.819	1.00	58.32
3326	CD2	LEU	671	23.606	40.677	39.673	1.00	59.37
3327	C	LEU	671	25.178	40.804	35.613	1.00	60.50
3328	O	LEU	671	24.076	41.295	35.377	1.00	61.24
3329	N	LEU	672	26.320	41.354	35.219	1.00	59.65
3330	CA	LEU	672	26.355	42.613	34.492	1.00	62.17
3331	CB	LEU	672	27.128	43.650	35.309	1.00	60.10
3332	CG	LEU	672	26.917	43.688	36.822	1.00	65.92
3333	CD1	LEU	672	27.728	44.819	37.407	1.00	60.54
3334	CD2	LEU	672	25.460	43.885	37.148	1.00	58.59
3335	C	LEU	672	27.027	42.456	33.131	1.00	62.29
3336	O	LEU	672	27.489	43.430	32.554	1.00	61.76
3337	N	SER	673	27.070	41.237	32.613	1.00	60.43
3338	CA	SER	673	27.732	40.980	31.342	1.00	60.60
3339	CB	SER	673	28.212	39.538	31.317	1.00	60.81
3340	OG	SER	673	27.281	38.718	31.987	1.00	56.49
3341	C	SER	673	26.949	41.280	30.074	1.00	60.41
3342	O	SER	673	27.542	41.502	29.020	1.00	60.96
3343	N	SER	674	25.625	41.267	30.160	1.00	62.26
3344	CA	SER	674	24.800	41.565	28.995	1.00	62.20
3345	CB	SER	674	24.359	40.281	28.298	1.00	61.34
3346	OG	SER	674	23.730	39.420	29.221	1.00	62.88
3347	C	SER	674	23.581	42.371	29.402	1.00	60.51
3348	O	SER	674	22.904	42.050	30.376	1.00	62.02
3349	N	VAL	675	23.321	43.432	28.653	1.00	61.79
3350	CA	VAL	675	22.190	44.299	28.911	1.00	61.63
3351	CB	VAL	675	22.670	45.712	29.194	1.00	59.56
3352	CG1	VAL	675	23.388	45.748	30.517	1.00	62.21
3353	CG2	VAL	675	23.598	46.164	28.078	1.00	63.23
3354	C	VAL	675	21.325	44.320	27.658	1.00	62.05
3355	O	VAL	675	21.757	43.861	26.603	1.00	62.28
3356	N	PRO	676	20.077	44.817	27.764	1.00	60.51
3357	CD	PRO	676	19.330	45.132	28.991	1.00	63.50

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3358	CA	PRO	676	19.191	44.880	26.593	1.00	62.22
	3359	CB	PRO	676	17.896	45.494	27.156	1.00	58.53
	3360	CG	PRO	676	18.322	46.117	28.488	1.00	60.68
10	3361	C	PRO	676	19.839	45.746	25.514	1.00	58.14
	3362	O	PRO	676	20.824	46.435	25.792	1.00	61.96
	3363	N	LYS	677	19.309	45.710	24.293	1.00	60.64
15	3364	CA	LYS	677	19.906	46.501	23.215	1.00	59.47
	3365	CB	LYS	677	19.025	46.521	21.970	1.00	61.69
	3366	CG	LYS	677	19.782	46.912	20.707	1.00	61.32
20	3367	CD	LYS	677	18.832	47.051	19.514	1.00	61.48
	3368	CE	LYS	677	19.604	47.129	18.198	1.00	62.13
	3369	NZ	LYS	677	20.435	45.908	17.952	1.00	60.25
25	3370	C	LYS	677	20.145	47.929	23.686	1.00	59.29
	3371	O	LYS	677	21.248	48.235	24.158	1.00	63.94
	3372	N	ASP	678	19.129	48.796	23.580	1.00	61.98
30	3373	CA	ASP	678	19.302	50.178	24.028	1.00	61.19
	3374	CB	ASP	678	18.178	51.083	23.506	1.00	60.11
	3375	CG	ASP	678	18.515	52.582	23.647	1.00	60.40
35	3376	OD1	ASP	678	18.311	53.325	22.652	1.00	60.21
	3377	OD2	ASP	678	18.980	53.011	24.745	1.00	61.19
	3378	C	ASP	678	19.395	50.284	25.558	1.00	61.02
40	3379	O	ASP	678	18.592	50.955	26.210	1.00	61.94
	3380	N	GLY	679	20.398	49.604	26.108	1.00	58.42
	3381	CA	GLY	679	20.649	49.605	27.534	1.00	56.97
45	3382	C	GLY	679	19.449	49.444	28.438	1.00	56.85
	3383	O	GLY	679	18.362	49.031	28.028	1.00	59.44
	3384	N	LEU	680	19.674	49.788	29.696	1.00	63.29
50	3385	CA	LEU	680	18.655	49.704	30.727	1.00	62.45
	3386	CB	LEU	680	19.297	49.181	32.017	1.00	64.86
	3387	CG	LEU	680	20.118	47.895	31.832	1.00	59.84
55	3388	CD1	LEU	680	20.946	47.595	33.068	1.00	59.62
	3389	CD2	LEU	680	19.181	46.760	31.543	1.00	61.01
	3390	C	LEU	680	18.056	51.090	30.955	1.00	60.58
55	3391	O	LEU	680	18.433	52.063	30.298	1.00	62.60
	3392	N	LYS	681	17.120	51.174	31.888	1.00	62.27
	3393	CA	LYS	681	16.486	52.441	32.197	1.00	63.23
	3394	CB	LYS	681	15.146	52.211	32.901	1.00	59.95

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3395	CG	LYS	681	14.188	51.417	32.034	1.00	60.87
	3396	CD	LYS	681	12.837	51.183	32.665	1.00	61.02
	3397	CE	LYS	681	12.004	50.295	31.740	1.00	64.07
10	3398	NZ	LYS	681	10.616	50.060	32.218	1.00	58.77
	3399	C	LYS	681	17.414	53.242	33.072	1.00	60.18
	3400	O	LYS	681	17.373	54.462	33.069	1.00	63.10
15	3401	N	SER	682	18.278	52.554	33.802	1.00	60.92
	3402	CA	SER	682	19.214	53.240	34.681	1.00	62.50
	3403	CB	SER	682	18.953	52.786	36.113	1.00	62.86
20	3404	OG	SER	682	17.564	52.589	36.296	1.00	61.69
	3405	C	SER	682	20.682	52.993	34.272	1.00	58.65
	3406	O	SER	682	21.558	52.781	35.120	1.00	60.76
25	3407	N	GLN	683	20.924	53.053	32.961	1.00	60.04
	3408	CA	GLN	683	22.241	52.840	32.348	1.00	61.19
	3409	CB	GLN	683	22.156	53.127	30.850	1.00	59.58
30	3410	CG	GLN	683	23.397	52.757	30.056	1.00	62.33
	3411	CD	GLN	683	23.606	51.259	29.955	1.00	62.33
	3412	OE1	GLN	683	22.651	50.502	29.759	1.00	62.13
35	3413	NE2	GLN	683	24.858	50.823	30.065	1.00	61.30
	3414	C	GLN	683	23.397	53.655	32.934	1.00	61.70
	3415	O	GLN	683	24.561	53.335	32.719	1.00	62.18
40	3416	N	GLU	684	23.083	54.710	33.666	1.00	64.02
	3417	CA	GLU	684	24.117	55.539	34.257	1.00	60.92
	3418	CB	GLU	684	23.541	56.904	34.590	1.00	62.70
45	3419	CG	GLU	684	22.396	56.780	35.574	1.00	62.30
	3420	CD	GLU	684	21.884	58.112	36.063	1.00	61.33
	3421	OE1	GLU	684	21.260	58.120	37.153	1.00	61.85
50	3422	OE2	GLU	684	22.092	59.135	35.363	1.00	62.66
	3423	C	GLU	684	24.582	54.867	35.534	1.00	61.21
	3424	O	GLU	684	25.741	54.979	35.924	1.00	63.65
55	3425	N	LEU	685	23.659	54.181	36.197	1.00	62.46
	3426	CA	LEU	685	23.992	53.487	37.429	1.00	60.48
	3427	CB	LEU	685	22.731	53.265	38.269	1.00	62.31
60	3428	CG	LEU	685	22.992	53.036	39.764	1.00	59.19
	3429	CD1	LEU	685	23.700	54.245	40.360	1.00	59.86
	3430	CD2	LEU	685	21.684	52.795	40.485	1.00	61.02
65	3431	C	LEU	685	24.657	52.148	37.086	1.00	61.95

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3432	O	LEU	685	25.524	51.662	37.804	1.00	61.31
	3433	N	PHE	686	24.264	51.566	35.964	1.00	60.07
	3434	CA	PHE	686	24.832	50.302	35.560	1.00	60.10
10	3435	CB	PHE	686	24.147	49.785	34.311	1.00	61.65
	3436	CG	PHE	686	24.500	48.372	33.990	1.00	62.45
	3437	CD1	PHE	686	24.148	47.352	34.860	1.00	58.40
15	3438	CD2	PHE	686	25.204	48.057	32.839	1.00	57.88
	3439	CE1	PHE	686	24.493	46.038	34.589	1.00	58.59
	3440	CE2	PHE	686	25.558	46.741	32.558	1.00	63.31
20	3441	CZ	PHE	686	25.201	45.733	33.433	1.00	61.15
	3442	C	PHE	686	26.321	50.423	35.287	1.00	61.88
	3443	O	PHE	686	27.150	49.890	36.038	1.00	60.58
25	3444	N	ASP	687	26.657	51.113	34.199	1.00	62.94
	3445	CA	ASP	687	28.048	51.291	33.817	1.00	61.00
	3446	CB	ASP	687	28.171	52.397	32.776	1.00	59.08
30	3447	CG	ASP	687	27.327	52.131	31.555	1.00	63.32
	3448	OD1	ASP	687	27.089	50.940	31.271	1.00	59.10
	3449	OD2	ASP	687	26.914	53.098	30.875	1.00	63.48
35	3450	C	ASP	687	28.853	51.645	35.051	1.00	60.66
	3451	O	ASP	687	29.988	51.203	35.213	1.00	60.12
	3452	N	GLU	688	28.238	52.424	35.934	1.00	62.70
40	3453	CA	GLU	688	28.869	52.872	37.172	1.00	64.06
	3454	CB	GLU	688	27.967	53.930	37.803	1.00	59.69
	3455	CG	GLU	688	28.530	54.718	38.963	1.00	60.90
45	3456	CD	GLU	688	27.609	55.883	39.319	1.00	59.61
	3457	OE1	GLU	688	27.607	56.905	38.575	1.00	59.94
	3458	OE2	GLU	688	26.871	55.765	40.328	1.00	61.24
50	3459	C	GLU	688	29.137	51.726	38.164	1.00	62.60
	3460	O	GLU	688	30.199	51.659	38.784	1.00	62.63
	3461	N	ILE	689	28.166	50.833	38.314	1.00	61.42
55	3462	CA	ILE	689	28.296	49.691	39.207	1.00	64.18
	3463	CB	ILE	689	26.919	49.043	39.453	1.00	57.30
	3464	CG2	ILE	689	27.080	47.686	40.125	1.00	62.29
55	3465	CG1	ILE	689	26.055	49.980	40.297	1.00	63.30
	3466	CD1	ILE	689	24.668	49.458	40.545	1.00	63.34
	3467	C	ILE	689	29.235	48.654	38.590	1.00	62.15
	3468	O	ILE	689	30.079	48.071	39.276	1.00	59.58

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5 3469	N	ARG	690	29.083	48.416	37.290	1.00	63.61
	3470	CA	ARG	690	29.938	47.455	1.00	64.65
	3471	CB	ARG	690	29.619	47.429	1.00	61.26
10 3472	CG	ARG	690	30.319	46.331	34.331	1.00	60.27
	3473	CD	ARG	690	29.665	46.159	1.00	61.69
	3474	NE	ARG	690	30.153	44.983	1.00	64.60
	3475	CZ	ARG	690	31.331	44.907	1.00	64.30
15 3476	NH1	ARG	690	32.158	45.946	31.657	1.00	61.69
	3477	NH2	ARG	690	31.682	43.793	1.00	61.35
	3478	C	ARG	690	31.387	47.863	1.00	62.11
20 3479	O	ARG	690	32.208	47.070	37.268	1.00	63.96
	3480	N	MET	691	31.690	49.118	1.00	58.67
	3481	CA	MET	691	33.029	49.642	1.00	62.38
	3482	CB	MET	691	33.015	51.144	1.00	63.73
25 3483	CG	MET	691	34.366	51.723	36.003	1.00	63.05
	3484	SD	MET	691	35.189	50.799	1.00	60.35
	3485	CE	MET	691	36.714	50.382	1.00	57.09
30 3486	C	MET	691	33.533	49.367	38.106	1.00	61.62
	3487	O	MET	691	34.653	48.907	1.00	60.31
	3488	N	THR	692	32.691	49.633	1.00	61.56
	3489	CA	THR	692	33.053	49.428	1.00	59.70
35 3490	CB	THR	692	31.899	49.838	41.404	1.00	61.08
	3491	OG1	THR	692	31.493	51.167	1.00	61.61
	3492	CG2	THR	692	32.331	49.794	1.00	61.81
40 3493	C	THR	692	33.478	47.997	40.837	1.00	61.92
	3494	O	THR	692	34.349	47.799	1.00	59.04
	3495	N	TYR	693	32.850	47.013	1.00	58.91
	3496	CA	TYR	693	33.183	45.605	1.00	59.83
45 3497	CB	TYR	693	31.961	44.711	40.241	1.00	59.81
	3498	CG	TYR	693	31.053	44.801	1.00	63.50
	3499	CD1	TYR	693	31.565	44.640	1.00	59.52
50 3500	CE1	TYR	693	30.757	44.793	43.844	1.00	63.13
	3501	CD2	TYR	693	29.703	45.109	1.00	59.74
	3502	CE2	TYR	693	28.892	45.259	1.00	61.29
	3503	CZ	TYR	693	29.428	45.101	1.00	62.95
55 3504	OH	TYR	693	28.625	45.264	44.760	1.00	60.97
	3505	C	TYR	693	34.310	45.138	1.00	62.66

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3506	O	TYR	693	34.856	44.059	39.732	1.00	60.97
	3507	N	ILE	694	34.648	45.955	38.536	1.00	62.91
	3508	CA	ILE	694	35.766	45.651	37.661	1.00	60.76
10	3509	CB	ILE	694	35.726	46.450	36.347	1.00	63.35
	3510	CG2	ILE	694	37.057	46.305	35.611	1.00	58.86
	3511	CG1	ILE	694	34.570	45.956	35.480	1.00	59.03
15	3512	CD1	ILE	694	34.524	46.568	34.109	1.00	64.66
	3513	C	ILE	694	36.947	46.106	38.496	1.00	59.29
	3514	O	ILE	694	37.976	45.450	38.548	1.00	59.81
20	3515	N	LYS	695	36.788	47.235	39.171	1.00	60.10
	3516	CA	LYS	695	37.850	47.718	40.031	1.00	59.42
	3517	CB	LYS	695	37.530	49.111	40.577	1.00	62.71
25	3518	CG	LYS	695	37.525	50.194	39.543	1.00	56.74
	3519	CD	LYS	695	37.579	51.556	40.199	1.00	62.01
	3520	CE	LYS	695	37.453	52.666	39.170	1.00	62.05
30	3521	NZ	LYS	695	37.650	54.002	39.778	1.00	58.55
	3522	C	LYS	695	37.996	46.741	41.193	1.00	60.49
	3523	O	LYS	695	39.071	46.578	41.744	1.00	58.83
35	3524	N	GLU	696	36.906	46.084	41.559	1.00	58.96
	3525	CA	GLU	696	36.924	45.135	42.663	1.00	63.14
	3526	CB	GLU	696	35.489	44.813	43.080	1.00	62.85
40	3527	CG	GLU	696	35.338	44.392	44.513	1.00	61.99
	3528	CD	GLU	696	35.888	45.410	45.497	1.00	62.60
	3529	OE1	GLU	696	35.609	46.616	45.353	1.00	60.89
45	3530	OE2	GLU	696	36.596	44.999	46.438	1.00	59.40
	3531	C	GLU	696	37.668	43.855	42.273	1.00	63.03
	3532	O	GLU	696	38.281	43.198	43.120	1.00	61.00
50	3533	N	LEU	697	37.605	43.507	40.990	1.00	61.52
	3534	CA	LEU	697	38.279	42.324	40.487	1.00	58.74
	3535	CB	LEU	697	37.830	42.018	39.057	1.00	58.36
55	3536	CG	LEU	697	38.438	40.757	38.439	1.00	63.54
	3537	CD1	LEU	697	37.948	39.560	39.208	1.00	57.14
	3538	CD2	LEU	697	38.058	40.623	36.972	1.00	63.58
55	3539	C	LEU	697	39.766	42.633	40.499	1.00	60.87
	3540	O	LEU	697	40.599	41.748	40.683	1.00	64.34
	3541	N	GLY	698	40.087	43.907	40.303	1.00	63.62
	3542	CA	GLY	698	41.472	44.331	40.285	1.00	60.55

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
3543	C	GLY	698	42.053	44.398	41.677	1.00	61.55
3544	O	GLY	698	43.259	44.268	41.877	1.00	58.62
3545	N	LYS	699	41.180	44.621	42.644	1.00	60.41
3546	CA	LYS	699	41.596	44.689	44.027	1.00	61.47
3547	CB	LYS	699	40.437	45.189	44.903	1.00	62.58
3548	CG	LYS	699	40.251	46.712	44.942	1.00	64.44
3549	CD	LYS	699	39.111	47.088	45.889	1.00	59.70
3550	CE	LYS	699	39.375	48.368	46.707	1.00	60.92
3551	NZ	LYS	699	38.986	49.663	46.056	1.00	62.69
3552	C	LYS	699	42.000	43.284	44.447	1.00	64.59
3553	O	LYS	699	43.044	43.077	45.063	1.00	59.56
3554	N	ALA	700	41.161	42.322	44.080	1.00	58.13
3555	CA	ALA	700	41.376	40.927	44.415	1.00	62.66
3556	CB	ALA	700	40.219	40.103	43.908	1.00	59.89
3557	C	ALA	700	42.678	40.387	43.861	1.00	60.42
3558	O	ALA	700	43.430	39.743	44.577	1.00	61.59
3559	N	ILE	701	42.937	40.662	42.585	1.00	60.42
3560	CA	ILE	701	44.141	40.201	41.898	1.00	63.95
3561	CB	ILE	701	44.105	40.611	40.416	1.00	61.37
3562	CG2	ILE	701	45.396	40.224	39.742	1.00	65.93
3563	CG1	ILE	701	42.921	39.939	39.717	1.00	60.90
3564	CD1	ILE	701	42.697	40.405	38.275	1.00	59.90
3565	C	ILE	701	45.465	40.675	42.514	1.00	61.05
3566	O	ILE	701	46.455	39.931	42.518	1.00	62.71
3567	N	VAL	702	45.495	41.901	43.030	1.00	64.20
3568	CA	VAL	702	46.723	42.409	43.637	1.00	61.51
3569	CB	VAL	702	46.690	43.949	43.841	1.00	61.28
3570	CG1	VAL	702	46.285	44.645	42.546	1.00	61.75
3571	CG2	VAL	702	45.753	44.305	44.983	1.00	63.42
3572	C	VAL	702	46.964	41.753	44.995	1.00	62.93
3573	O	VAL	702	48.101	41.598	45.432	1.00	62.05
3574	N	LYS	703	45.894	41.357	45.665	1.00	61.37
3575	CA	LYS	703	46.057	40.741	46.967	1.00	62.89
3576	CB	LYS	703	44.714	40.683	47.705	1.00	58.24
3577	CG	LYS	703	44.851	40.816	49.215	1.00	61.67
3578	CD	LYS	703	45.460	39.557	49.830	1.00	63.57
3579	CE	LYS	703	46.410	39.869	50.986	1.00	57.61

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3580	NZ	LYS	703	46.656	38.664	51.838	1.00	61.16
	3581	C	LYS	703	46.645	39.355	46.776	1.00	60.39
	3582	O	LYS	703	46.974	38.668	47.731	1.00	61.26
10	3583	N	ARG	704	46.790	38.951	45.523	1.00	62.02
	3584	CA	ARG	704	47.369	37.649	45.214	1.00	61.58
	3585	CB	ARG	704	46.408	36.817	44.368	1.00	61.15
15	3586	CG	ARG	704	45.272	36.177	45.112	1.00	66.70
	3587	CD	ARG	704	44.871	34.956	44.350	1.00	62.98
	3588	NE	ARG	704	45.731	34.788	43.185	1.00	58.04
20	3589	CZ	ARG	704	45.973	33.619	42.601	1.00	65.26
	3590	NH1	ARG	704	45.422	32.513	43.080	1.00	60.05
	3591	NH2	ARG	704	46.761	33.552	41.538	1.00	60.69
25	3592	C	ARG	704	48.686	37.792	44.445	1.00	62.07
	3593	O	ARG	704	49.779	37.725	45.029	1.00	60.23
	3594	N	GLU	705	48.555	37.997	43.130	1.00	61.20
30	3595	CA	GLU	705	49.686	38.134	42.212	1.00	61.45
	3596	CB	GLU	705	49.179	38.271	40.776	1.00	59.83
	3597	CG	GLU	705	49.038	36.941	40.015	1.00	61.58
35	3598	CD	GLU	705	48.539	35.764	40.875	1.00	62.88
	3599	OE1	GLU	705	47.511	35.908	41.595	1.00	61.37
	3600	OE2	GLU	705	49.181	34.685	40.806	1.00	62.83
40	3601	C	GLU	705	50.601	39.296	42.542	1.00	60.29
	3602	O	GLU	705	50.212	40.468	42.446	1.00	61.23
	3603	N	GLY	706	51.832	38.935	42.896	1.00	60.12
45	3604	CA	GLY	706	52.855	39.883	43.288	1.00	62.85
	3605	C	GLY	706	53.083	41.191	42.556	1.00	58.46
	3606	O	GLY	706	52.603	42.244	42.991	1.00	60.65
50	3607	N	ASN	707	53.818	41.141	41.449	1.00	62.51
	3608	CA	ASN	707	54.158	42.366	40.729	1.00	63.30
	3609	CB	ASN	707	55.516	42.196	40.013	1.00	60.74
55	3610	CG	ASN	707	55.676	40.835	39.356	1.00	60.19
	3611	OD1	ASN	707	55.354	39.797	39.950	1.00	59.76
	3612	ND2	ASN	707	56.195	40.833	38.128	1.00	59.34
55	3613	C	ASN	707	53.134	42.993	39.792	1.00	59.87
	3614	O	ASN	707	52.054	42.451	39.569	1.00	63.44
	3615	N	SER	708	53.501	44.161	39.265	1.00	60.90
	3616	CA	SER	708	52.647	44.950	38.382	1.00	58.16

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5 3617	CB	SER	708	53.218	46.366	38.244	1.00	62.09
3618	OG	SER	708	53.403	46.974	39.516	1.00	61.85
3619	C	SER	708	52.432	44.354	36.998	1.00	61.28
10 3620	O	SER	708	51.400	44.607	36.372	1.00	58.94
3621	N	SER	709	53.393	43.567	36.516	1.00	61.19
3622	CA	SER	709	53.266	42.952	35.193	1.00	59.82
3623	CB	SER	709	54.650	42.527	34.665	1.00	62.14
15 3624	OG	SER	709	54.658	42.353	33.249	1.00	61.67
3625	C	SER	709	52.338	41.743	35.318	1.00	59.05
3626	O	SER	709	51.508	41.479	34.442	1.00	63.30
20 3627	N	GLN	710	52.481	41.022	36.426	1.00	63.44
3628	CA	GLN	710	51.652	39.851	36.691	1.00	59.41
3629	CB	GLN	710	52.289	39.036	37.833	1.00	63.27
3630	CG	GLN	710	53.572	38.329	37.354	1.00	60.06
25 3631	CD	GLN	710	54.362	37.611	38.453	1.00	57.38
3632	OE1	GLN	710	53.781	37.012	39.369	1.00	60.97
3633	NE2	GLN	710	55.701	37.647	38.348	1.00	63.13
30 3634	C	GLN	710	50.209	40.281	37.010	1.00	62.98
3635	O	GLN	710	49.250	39.584	36.667	1.00	61.41
3636	N	ASN	711	50.087	41.451	37.641	1.00	59.07
3637	CA	ASN	711	48.815	42.048	38.017	1.00	59.32
35 3638	CB	ASN	711	49.053	43.439	38.610	1.00	62.53
3639	CG	ASN	711	49.400	43.398	40.096	1.00	65.70
3640	OD1	ASN	711	49.886	44.388	40.663	1.00	59.52
40 3641	ND2	ASN	711	49.140	42.259	40.736	1.00	62.62
3642	C	ASN	711	47.918	42.167	36.792	1.00	61.19
3643	O	ASN	711	46.796	41.644	36.778	1.00	59.41
45 3644	N	TRP	712	48.418	42.850	35.762	1.00	60.32
3645	CA	TRP	712	47.660	43.044	34.534	1.00	65.58
3646	CB	TRP	712	48.270	44.168	33.711	1.00	59.75
3647	CG	TRP	712	48.272	45.426	34.444	1.00	58.80
50 3648	CD2	TRP	712	47.148	46.271	34.668	1.00	64.37
3649	CE2	TRP	712	47.577	47.322	35.506	1.00	59.23
3650	CE3	TRP	712	45.812	46.240	34.245	1.00	62.90
55 3651	CD1	TRP	712	49.313	45.976	35.124	1.00	62.87
3652	NE1	TRP	712	48.905	47.118	35.770	1.00	62.24
3653	CZ2	TRP	712	46.719	48.335	35.935	1.00	60.25

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3654	CZ3	TRP	712	44.954	47.247	34.672	1.00	61.54
	3655	CH2	TRP	712	45.413	48.281	35.511	1.00	58.28
	3656	C	TRP	712	47.538	41.811	33.663	1.00	61.45
10	3657	O	TRP	712	46.531	41.623	32.992	1.00	63.89
	3658	N	GLN	713	48.561	40.974	33.646	1.00	62.44
	3659	CA	GLN	713	48.493	39.778	32.823	1.00	60.84
15	3660	CB	GLN	713	49.865	39.088	32.761	1.00	59.49
	3661	CG	GLN	713	50.495	39.114	31.371	1.00	61.40
	3662	CD	GLN	713	49.624	38.414	30.336	1.00	60.98
20	3663	OE1	GLN	713	49.306	38.980	29.285	1.00	60.97
	3664	NE2	GLN	713	49.232	37.173	30.629	1.00	62.19
	3665	C	GLN	713	47.446	38.847	33.420	1.00	64.17
25	3666	O	GLN	713	46.843	38.037	32.722	1.00	62.77
	3667	N	ARG	714	47.242	38.993	34.724	1.00	60.50
	3668	CA	ARG	714	46.276	38.203	35.481	1.00	60.81
30	3669	CB	ARG	714	46.560	38.352	36.978	1.00	61.22
	3670	CG	ARG	714	45.609	37.613	37.897	1.00	60.90
	3671	CD	ARG	714	45.858	36.130	37.894	1.00	60.47
35	3672	NE	ARG	714	44.999	35.455	38.858	1.00	60.72
	3673	CZ	ARG	714	44.777	34.145	38.860	1.00	62.42
	3674	NH1	ARG	714	45.358	33.382	37.943	1.00	57.63
40	3675	NH2	ARG	714	43.967	33.601	39.762	1.00	61.24
	3676	C	ARG	714	44.877	38.722	35.174	1.00	61.77
	3677	O	ARG	714	43.930	37.949	35.007	1.00	61.51
45	3678	N	PHE	715	44.765	40.044	35.107	1.00	59.93
	3679	CA	PHE	715	43.502	40.691	34.809	1.00	62.80
	3680	CB	PHE	715	43.630	42.203	34.932	1.00	61.91
50	3681	CG	PHE	715	42.335	42.909	34.749	1.00	63.38
	3682	CD1	PHE	715	41.340	42.779	35.706	1.00	62.36
	3683	CD2	PHE	715	42.062	43.610	33.581	1.00	62.07
55	3684	CE1	PHE	715	40.091	43.323	35.504	1.00	60.49
	3685	CE2	PHE	715	40.815	44.162	33.365	1.00	62.56
	3686	CZ	PHE	715	39.823	44.017	34.328	1.00	61.44
60	3687	C	PHE	715	43.046	40.353	33.395	1.00	60.17
	3688	O	PHE	715	41.849	40.288	33.115	1.00	59.69
	3689	N	TYR	716	44.017	40.157	32.507	1.00	61.56
65	3690	CA	TYR	716	43.749	39.820	31.116	1.00	60.99

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	3691	CB	TYR	716	45.043	39.870	30.297	1.00	62.72
	3692	CG	TYR	716	44.810	39.609	28.828	1.00	61.29
	3693	CD1	TYR	716	44.115	40.530	28.047	1.00	57.90
10	3694	CE1	TYR	716	43.790	40.253	26.728	1.00	62.63
	3695	CD2	TYR	716	45.188	38.399	28.242	1.00	65.06
	3696	CE2	TYR	716	44.866	38.111	26.923	1.00	60.30
15	3697	CZ	TYR	716	44.161	39.044	26.172	1.00	62.23
	3698	OH	TYR	716	43.798	38.768	24.870	1.00	58.39
	3699	C	TYR	716	43.157	38.419	31.036	1.00	62.09
20	3700	O	TYR	716	42.085	38.213	30.469	1.00	60.05
	3701	N	GLN	717	43.875	37.460	31.611	1.00	62.41
	3702	CA	GLN	717	43.449	36.071	31.623	1.00	60.55
25	3703	CB	GLN	717	44.409	35.222	32.465	1.00	59.06
	3704	CG	GLN	717	45.855	35.166	31.978	1.00	60.27
	3705	CD	GLN	717	46.758	34.357	32.919	1.00	60.87
30	3706	OE1	GLN	717	46.844	34.639	34.124	1.00	61.07
	3707	NE2	GLN	717	47.437	33.352	32.369	1.00	62.22
	3708	C	GLN	717	42.048	35.931	32.194	1.00	59.73
35	3709	O	GLN	717	41.156	35.383	31.545	1.00	64.26
	3710	N	LEU	718	41.867	36.428	33.415	1.00	58.62
	3711	CA	LEU	718	40.582	36.348	34.101	1.00	60.65
40	3712	CB	LEU	718	40.708	36.899	35.530	1.00	61.42
	3713	CG	LEU	718	41.661	36.158	36.487	1.00	61.76
	3714	CD1	LEU	718	41.717	36.889	37.809	1.00	60.77
45	3715	CD2	LEU	718	41.210	34.721	36.701	1.00	59.74
	3716	C	LEU	718	39.427	37.034	33.375	1.00	59.70
	3717	O	LEU	718	38.330	36.495	33.327	1.00	60.84
50	3718	N	THR	719	39.661	38.211	32.812	1.00	62.09
	3719	CA	THR	719	38.608	38.925	32.095	1.00	59.89
	3720	CB	THR	719	38.985	40.387	31.900	1.00	63.01
55	3721	OG1	THR	719	40.248	40.465	31.237	1.00	63.25
	3722	CG2	THR	719	39.087	41.082	33.240	1.00	61.82
	3723	C	THR	719	38.329	38.291	30.733	1.00	61.35
55	3724	O	THR	719	37.349	38.622	30.062	1.00	61.10
	3725	N	LYS	720	39.203	37.371	30.341	1.00	62.98
	3726	CA	LYS	720	39.074	36.651	29.079	1.00	61.71
	3727	CB	LYS	720	40.460	36.209	28.588	1.00	62.48

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3728	CG	LYS	720	40.500	35.805	27.128	1.00	58.53
	3729	CD	LYS	720	40.038	36.972	26.251	1.00	59.89
	3730	CE	LYS	720	39.616	36.524	24.842	1.00	58.48
10	3731	NZ	LYS	720	38.772	37.570	24.209	1.00	60.64
	3732	C	LYS	720	38.184	35.430	29.331	1.00	61.74
	3733	O	LYS	720	37.479	34.962	28.438	1.00	61.10
15	3734	N	LEU	721	38.228	34.923	30.560	1.00	61.01
	3735	CA	LEU	721	37.417	33.776	30.938	1.00	64.67
	3736	CB	LEU	721	37.897	33.187	32.268	1.00	59.87
20	3737	CG	LEU	721	37.656	31.707	32.594	1.00	61.04
	3738	CD1	LEU	721	37.766	31.549	34.095	1.00	57.32
	3739	CD2	LEU	721	36.292	31.224	32.130	1.00	59.37
25	3740	C	LEU	721	35.983	34.277	31.078	1.00	62.25
	3741	O	LEU	721	35.031	33.533	30.860	1.00	57.52
	3742	N	LEU	722	35.830	35.540	31.455	1.00	62.01
30	3743	CA	LEU	722	34.503	36.113	31.591	1.00	62.92
	3744	CB	LEU	722	34.578	37.497	32.246	1.00	61.91
	3745	CG	LEU	722	34.841	37.559	33.754	1.00	58.92
35	3746	CD1	LEU	722	34.946	38.986	34.193	1.00	62.12
	3747	CD2	LEU	722	33.728	36.876	34.507	1.00	62.52
	3748	C	LEU	722	33.949	36.226	30.180	1.00	59.20
40	3749	O	LEU	722	32.883	35.697	29.854	1.00	60.43
	3750	N	ASP	723	34.714	36.911	29.344	1.00	60.22
	3751	CA	ASP	723	34.379	37.143	27.952	1.00	60.07
45	3752	CB	ASP	723	35.607	37.697	27.248	1.00	59.74
	3753	CG	ASP	723	35.437	39.115	26.832	1.00	60.94
	3754	OD1	ASP	723	34.869	39.890	27.626	1.00	63.82
50	3755	OD2	ASP	723	35.883	39.445	25.713	1.00	63.76
	3756	C	ASP	723	33.909	35.899	27.214	1.00	61.21
	3757	O	ASP	723	33.108	35.981	26.292	1.00	61.67
55	3758	N	SER	724	34.414	34.743	27.613	1.00	62.19
	3759	CA	SER	724	34.054	33.521	26.923	1.00	62.38
	3760	CB	SER	724	35.256	32.578	26.876	1.00	61.26
55	3761	OG	SER	724	35.743	32.308	28.175	1.00	62.27
	3762	C	SER	724	32.869	32.823	27.539	1.00	63.42
	3763	O	SER	724	32.419	31.785	27.054	1.00	60.80
	3764	N	MET	725	32.352	33.395	28.613	1.00	61.24

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	3765	CA	MET	725	31.209	32.794	29.265	1.00	60.73
	3766	CB	MET	725	30.955	33.461	30.608	1.00	62.85
	3767	CG	MET	725	30.460	32.506	31.654	1.00	63.01
10	3768	SD	MET	725	31.773	31.403	32.092	1.00	57.07
	3769	CE	MET	725	30.949	30.380	33.178	1.00	59.44
	3770	C	MET	725	30.008	32.987	28.352	1.00	59.13
15	3771	O	MET	725	29.022	32.254	28.437	1.00	62.11
	3772	N	HIS	726	30.105	33.973	27.465	1.00	58.55
	3773	CA	HIS	726	29.021	34.267	26.547	1.00	60.99
20	3774	CB	HIS	726	29.302	35.554	25.769	1.00	62.45
	3775	CG	HIS	726	29.036	36.801	26.557	1.00	59.03
	3776	CD2	HIS	726	27.909	37.248	27.161	1.00	60.25
25	3777	ND1	HIS	726	30.003	37.753	26.800	1.00	61.07
	3778	CE1	HIS	726	29.484	38.731	27.520	1.00	61.93
	3779	NE2	HIS	726	28.215	38.451	27.752	1.00	59.78
30	3780	C	HIS	726	28.773	33.116	25.601	1.00	58.35
	3781	O	HIS	726	27.638	32.696	25.438	1.00	61.58
	3782	N	GLU	727	29.816	32.571	24.993	1.00	62.79
35	3783	CA	GLU	727	29.574	31.461	24.086	1.00	60.53
	3784	CB	GLU	727	30.693	31.307	23.055	1.00	59.90
	3785	CG	GLU	727	32.005	30.809	23.578	1.00	57.32
40	3786	CD	GLU	727	32.838	30.187	22.473	1.00	59.99
	3787	OE1	GLU	727	34.057	30.013	22.680	1.00	62.44
	3788	OE2	GLU	727	32.275	29.862	21.400	1.00	63.27
45	3789	C	GLU	727	29.351	30.138	24.791	1.00	59.24
	3790	O	GLU	727	28.779	29.233	24.203	1.00	62.98
	3791	N	VAL	728	29.812	29.992	26.029	1.00	60.19
50	3792	CA	VAL	728	29.546	28.732	26.721	1.00	58.29
	3793	CB	VAL	728	30.493	28.481	27.956	1.00	58.87
	3794	CG1	VAL	728	31.261	29.728	28.304	1.00	60.81
55	3795	CG2	VAL	728	29.694	28.002	29.152	1.00	61.95
	3796	C	VAL	728	28.082	28.825	27.145	1.00	59.41
	3797	O	VAL	728	27.335	27.848	27.046	1.00	61.38
	3798	N	VAL	729	27.670	30.014	27.585	1.00	59.91
	3799	CA	VAL	729	26.283	30.238	27.971	1.00	60.73
	3800	CB	VAL	729	26.072	31.664	28.504	1.00	63.53
	3801	CG1	VAL	729	24.602	32.062	28.406	1.00	62.52

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
3802	CG2	VAL	729	26.513	31.725	29.946	1.00	62.40
3803	C	VAL	729	25.397	30.004	26.749	1.00	62.11
3804	O	VAL	729	24.279	29.493	26.868	1.00	58.35
3805	N	GLU	730	25.894	30.372	25.571	1.00	59.30
3806	CA	GLU	730	25.133	30.146	24.347	1.00	61.37
3807	CB	GLU	730	25.940	30.546	23.125	1.00	57.56
3808	CG	GLU	730	25.202	31.467	22.199	1.00	61.79
3809	CD	GLU	730	25.875	31.569	20.859	1.00	62.47
3810	OE1	GLU	730	27.039	32.032	20.811	1.00	62.43
3811	OE2	GLU	730	25.235	31.178	19.858	1.00	61.70
3812	C	GLU	730	24.832	28.660	24.267	1.00	60.90
3813	O	GLU	730	23.701	28.244	24.449	1.00	63.19
3814	N	ASN	731	25.864	27.866	24.013	1.00	61.88
3815	CA	ASN	731	25.729	26.416	23.919	1.00	63.18
3816	CB	ASN	731	27.109	25.761	23.859	1.00	56.96
3817	CG	ASN	731	27.516	25.393	22.449	1.00	61.50
3818	OD1	ASN	731	26.909	24.515	21.808	1.00	59.01
3819	ND2	ASN	731	28.552	26.059	21.953	1.00	62.29
3820	C	ASN	731	24.927	25.773	25.045	1.00	62.97
3821	O	ASN	731	24.251	24.772	24.834	1.00	60.93
3822	N	LEU	732	25.002	26.330	26.246	1.00	59.50
3823	CA	LEU	732	24.241	25.737	27.326	1.00	57.74
3824	CB	LEU	732	24.826	26.120	28.668	1.00	61.00
3825	CG	LEU	732	25.964	25.172	29.078	1.00	60.69
3826	CD1	LEU	732	26.278	25.584	30.458	1.00	63.28
3827	CD2	LEU	732	25.589	23.663	29.058	1.00	63.30
3828	C	LEU	732	22.761	26.089	27.240	1.00	61.98
3829	O	LEU	732	21.912	25.269	27.574	1.00	63.87
3830	N	LEU	733	22.456	27.294	26.762	1.00	63.36
3831	CA	LEU	733	21.073	27.744	26.596	1.00	57.15
3832	CB	LEU	733	21.040	29.241	26.290	1.00	60.30
3833	CG	LEU	733	21.134	30.193	27.481	1.00	57.97
3834	CD1	LEU	733	21.471	31.571	26.956	1.00	62.48
3835	CD2	LEU	733	19.824	30.212	28.272	1.00	62.63
3836	C	LEU	733	20.354	26.997	25.470	1.00	63.32
3837	O	LEU	733	19.256	26.475	25.655	1.00	61.30
3838	N	ASN	734	20.965	26.972	24.292	1.00	57.57

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
3839	CA	ASN	734	20.376	26.285	23.159	1.00	59.44
3840	CB	ASN	734	21.363	26.277	21.994	1.00	57.94
3841	CG	ASN	734	21.671	27.682	21.495	1.00	59.18
3842	OD1	ASN	734	22.072	28.556	22.268	1.00	63.60
3843	ND2	ASN	734	21.476	27.908	20.202	1.00	63.41
3844	C	ASN	734	20.038	24.872	23.594	1.00	60.75
3845	O	ASN	734	18.904	24.423	23.453	1.00	62.53
3846	N	TYR	735	21.017	24.177	24.151	1.00	61.37
3847	CA	TYR	735	20.762	22.823	24.597	1.00	58.79
3848	CB	TYR	735	22.058	22.201	25.158	1.00	58.40
3849	CG	TYR	735	22.087	20.717	24.978	1.00	60.44
3850	CD1	TYR	735	21.309	19.890	25.780	1.00	60.76
3851	CE1	TYR	735	21.240	18.509	25.562	1.00	60.42
3852	CD2	TYR	735	22.815	20.134	23.938	1.00	61.19
3853	CE2	TYR	735	22.750	18.758	23.696	1.00	62.36
3854	CZ	TYR	735	21.961	17.950	24.519	1.00	59.04
3855	OH	TYR	735	21.899	16.583	24.313	1.00	58.73
3856	C	TYR	735	19.649	22.877	25.657	1.00	61.17
3857	O	TYR	735	18.858	21.945	25.790	1.00	63.18
3858	N	CYS	736	19.574	23.995	26.373	1.00	63.51
3859	CA	CYS	736	18.563	24.202	27.403	1.00	65.29
3860	CB	CYS	736	18.922	25.433	28.228	1.00	64.15
3861	SG	CYS	736	17.642	25.957	29.339	1.00	60.76
3862	C	CYS	736	17.183	24.389	26.779	1.00	63.45
3863	O	CYS	736	16.251	23.645	27.090	1.00	61.32
3864	N	PHE	737	17.061	25.391	25.906	1.00	59.77
3865	CA	PHE	737	15.808	25.688	25.209	1.00	61.17
3866	CB	PHE	737	16.014	26.792	24.175	1.00	59.61
3867	CG	PHE	737	16.348	28.129	24.764	1.00	58.80
3868	CD1	PHE	737	16.060	28.414	26.096	1.00	59.85
3869	CD2	PHE	737	16.924	29.119	23.979	1.00	61.58
3870	CE1	PHE	737	16.340	29.669	26.638	1.00	59.75
3871	CE2	PHE	737	17.207	30.374	24.510	1.00	61.15
3872	CZ	PHE	737	16.914	30.649	25.843	1.00	59.90
3873	C	PHE	737	15.280	24.462	24.484	1.00	61.86
3874	O	PHE	737	14.153	24.024	24.714	1.00	64.04
3875	N	GLN	738	16.108	23.932	23.590	1.00	60.57

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3876	CA	GLN	738	15.786	22.752	22.798	1.00	61.63
	3877	CB	GLN	738	17.078	22.181	22.220	1.00	62.59
	3878	CG	GLN	738	16.989	20.805	21.575	1.00	61.50
10	3879	CD	GLN	738	18.368	20.144	21.521	1.00	62.73
	3880	OE1	GLN	738	18.581	19.062	22.093	1.00	60.75
	3881	NE2	GLN	738	19.321	20.808	20.853	1.00	61.08
15	3882	C	GLN	738	15.043	21.677	23.591	1.00	62.87
	3883	O	GLN	738	13.970	21.235	23.180	1.00	62.00
	3884	N	THR	739	15.595	21.262	24.725	1.00	62.54
20	3885	CA	THR	739	14.937	20.228	25.513	1.00	62.00
	3886	CB	THR	739	15.883	19.572	26.529	1.00	61.40
	3887	OG1	THR	739	16.041	20.437	27.659	1.00	59.46
25	3888	CG2	THR	739	17.234	19.302	25.902	1.00	67.45
	3889	C	THR	739	13.721	20.740	26.282	1.00	60.54
	3890	O	THR	739	12.911	19.949	26.758	1.00	60.32
30	3891	N	PHE	740	13.589	22.049	26.433	1.00	60.26
	3892	CA	PHE	740	12.426	22.572	27.136	1.00	60.59
	3893	CB	PHE	740	12.645	24.013	27.586	1.00	60.53
35	3894	CG	PHE	740	11.387	24.682	28.073	1.00	60.33
	3895	CD1	PHE	740	10.976	24.543	29.399	1.00	60.24
	3896	CD2	PHE	740	10.591	25.417	27.196	1.00	60.88
40	3897	CE1	PHE	740	9.794	25.124	29.842	1.00	62.19
	3898	CE2	PHE	740	9.407	26.001	27.629	1.00	63.06
	3899	CZ	PHE	740	9.005	25.857	28.954	1.00	59.45
45	3900	C	PHE	740	11.269	22.562	26.161	1.00	62.20
	3901	O	PHE	740	10.102	22.514	26.560	1.00	60.22
	3902	N	LEU	741	11.619	22.631	24.877	1.00	61.98
50	3903	CA	LEU	741	10.650	22.665	23.783	1.00	61.09
	3904	CB	LEU	741	11.158	23.561	22.656	1.00	63.24
	3905	CG	LEU	741	11.286	25.053	22.919	1.00	57.80
55	3906	CD1	LEU	741	11.680	25.732	21.617	1.00	59.82
	3907	CD2	LEU	741	9.966	25.608	23.455	1.00	59.42
	3908	C	LEU	741	10.313	21.316	23.170	1.00	60.22
55	3909	O	LEU	741	9.748	21.267	22.079	1.00	59.13
	3910	N	ASP	742	10.662	20.230	23.845	1.00	61.37
	3911	CA	ASP	742	10.388	18.914	23.309	1.00	61.75
	3912	CB	ASP	742	11.679	18.315	22.733	1.00	62.29

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	3913	CG	ASP	742	11.476	16.916	22.145	1.00	59.85
	3914	OD1	ASP	742	12.450	16.354	21.576	1.00	62.02
	3915	OD2	ASP	742	10.348	16.378	22.253	1.00	63.60
10	3916	C	ASP	742	9.843	18.041	24.420	1.00	61.37
	3917	O	ASP	742	10.614	17.412	25.153	1.00	62.69
	3918	N	LYS	743	8.517	18.018	24.564	1.00	61.79
15	3919	CA	LYS	743	7.882	17.183	25.595	1.00	58.96
	3920	CB	LYS	743	6.381	17.501	25.727	1.00	62.19
	3921	CG	LYS	743	6.056	18.836	26.404	1.00	57.47
20	3922	CD	LYS	743	4.545	19.047	26.473	1.00	59.18
	3923	CE	LYS	743	4.180	20.313	27.232	1.00	61.36
	3924	NZ	LYS	743	2.699	20.507	27.295	1.00	57.73
25	3925	C	LYS	743	8.055	15.688	25.281	1.00	61.20
	3926	O	LYS	743	7.912	14.843	26.165	1.00	60.18
	3927	N	THR	744	8.366	15.380	24.020	1.00	59.67
30	3928	CA	THR	744	8.580	14.007	23.554	1.00	61.15
	3929	CB	THR	744	8.792	13.974	22.047	1.00	59.67
	3930	OG1	THR	744	7.881	14.890	21.426	1.00	62.19
35	3931	CG2	THR	744	8.550	12.574	21.513	1.00	63.96
	3932	C	THR	744	9.818	13.406	24.202	1.00	61.58
	3933	O	THR	744	9.976	12.195	24.261	1.00	62.58
40	3934	N	MET	745	10.711	14.279	24.646	1.00	57.60
	3935	CA	MET	745	11.933	13.887	25.334	1.00	62.60
	3936	CB	MET	745	12.982	14.976	25.147	1.00	59.01
45	3937	CG	MET	745	14.366	14.645	25.612	1.00	60.84
	3938	SD	MET	745	15.440	15.948	24.965	1.00	58.90
	3939	CE	MET	745	16.317	15.039	23.610	1.00	62.07
50	3940	C	MET	745	11.435	13.843	26.774	1.00	63.96
	3941	O	MET	745	11.973	13.137	27.629	1.00	64.77
	3942	N	SER	746	10.394	14.635	27.025	1.00	59.79
55	3943	CA	SER	746	9.744	14.657	28.326	1.00	60.83
	3944	CB	SER	746	9.149	13.249	28.576	1.00	61.05
	3945	OG	SER	746	8.512	13.111	29.842	1.00	61.76
	3946	C	SER	746	10.597	15.089	29.533	1.00	61.97
	3947	O	SER	746	10.576	14.408	30.545	1.00	61.88
	3948	N	ILE	747	11.322	16.207	29.443	1.00	60.50
	3949	CA	ILE	747	12.140	16.678	30.571	1.00	61.46

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	3950	CB	ILE	747	13.557	17.115	30.098	1.00	57.79
	3951	CG2	ILE	747	14.374	17.635	31.275	1.00	62.83
	3952	CG1	ILE	747	14.282	15.911	29.484	1.00	61.46
10	3953	CD1	ILE	747	15.664	16.211	28.976	1.00	65.11
	3954	C	ILE	747	11.441	17.829	31.318	1.00	63.68
	3955	O	ILE	747	11.166	18.891	30.747	1.00	62.48
15	3956	N	GLU	748	11.167	17.597	32.601	1.00	59.16
	3957	CA	GLU	748	10.457	18.546	33.466	1.00	62.34
	3958	CB	GLU	748	9.803	17.736	34.620	1.00	60.97
20	3959	CG	GLU	748	8.628	18.410	35.400	1.00	63.60
	3960	CD	GLU	748	7.998	17.505	36.516	1.00	59.56
	3961	OE1	GLU	748	8.753	16.918	37.340	1.00	61.60
25	3962	OE2	GLU	748	6.744	17.396	36.574	1.00	62.18
	3963	C	GLU	748	11.333	19.701	34.022	1.00	59.89
	3964	O	GLU	748	12.503	19.498	34.367	1.00	59.20
30	3965	N	PHE	749	10.781	20.913	34.046	1.00	62.20
	3966	CA	PHE	749	11.484	22.079	34.601	1.00	60.36
	3967	CB	PHE	749	11.773	23.202	33.571	1.00	63.43
35	3968	CG	PHE	749	12.801	22.827	32.506	1.00	62.31
	3969	CD1	PHE	749	12.604	21.790	31.624	1.00	63.18
	3970	CD2	PHE	749	13.948	23.639	32.305	1.00	58.27
40	3971	CE1	PHE	749	13.461	21.555	30.545	1.00	59.47
	3972	CE2	PHE	749	14.821	23.409	31.221	1.00	59.31
	3973	CZ	PHE	749	14.566	22.379	30.341	1.00	60.26
45	3974	C	PHE	749	10.491	22.634	35.646	1.00	57.34
	3975	O	PHE	749	9.296	22.348	35.598	1.00	62.05
	3976	N	PRO	750	10.971	23.425	36.612	1.00	61.11
50	3977	CD	PRO	750	12.322	23.572	37.178	1.00	62.36
	3978	CA	PRO	750	9.955	23.918	37.535	1.00	63.79
	3979	CB	PRO	750	10.745	24.124	38.834	1.00	59.84
55	3980	CG	PRO	750	12.072	24.510	38.341	1.00	61.92
	3981	C	PRO	750	9.283	25.174	37.042	1.00	61.44
	3982	O	PRO	750	9.000	25.325	35.852	1.00	61.38
55	3983	N	GLU	751	9.016	26.087	37.962	1.00	61.10
	3984	CA	GLU	751	8.375	27.335	37.604	1.00	59.57
	3985	CB	GLU	751	7.535	27.828	38.778	1.00	60.79
	3986	CG	GLU	751	6.534	26.804	39.190	1.00	60.87

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
3987	CD	GLU	751	5.716	26.358	38.013	1.00	58.45
3988	OE1	GLU	751	6.004	26.825	36.889	1.00	58.76
3989	OE2	GLU	751	4.768	25.564	38.205	1.00	62.99
3990	C	GLU	751	9.449	28.328	37.275	1.00	59.04
3991	O	GLU	751	9.644	28.698	36.115	1.00	63.48
3992	N	MET	752	10.154	28.736	38.319	1.00	62.70
3993	CA	MET	752	11.223	29.693	38.184	1.00	60.75
3994	CB	MET	752	12.241	29.499	39.306	1.00	60.00
3995	CG	MET	752	13.222	30.641	39.392	1.00	60.74
3996	SD	MET	752	12.305	32.203	39.387	1.00	61.02
3997	CE	MET	752	12.040	32.394	41.073	1.00	58.25
3998	C	MET	752	11.919	29.549	36.847	1.00	61.43
3999	O	MET	752	12.062	30.515	36.103	1.00	63.92
4000	N	LEU	753	12.329	28.326	36.537	1.00	61.53
4001	CA	LEU	753	13.044	28.081	35.307	1.00	63.94
4002	CB	LEU	753	13.749	26.729	35.370	1.00	61.07
4003	CG	LEU	753	15.278	26.834	35.432	1.00	59.22
4004	CD1	LEU	753	15.720	27.666	36.636	1.00	60.65
4005	CD2	LEU	753	15.870	25.436	35.488	1.00	56.88
4006	C	LEU	753	12.182	28.179	34.073	1.00	62.24
4007	O	LEU	753	12.539	28.882	33.138	1.00	61.75
4008	N	ALA	754	11.049	27.488	34.061	1.00	58.32
4009	CA	ALA	754	10.156	27.536	32.902	1.00	60.89
4010	CB	ALA	754	8.856	26.790	33.209	1.00	62.87
4011	C	ALA	754	9.851	28.995	32.581	1.00	60.33
4012	O	ALA	754	10.031	29.471	31.454	1.00	61.42
4013	N	GLU	755	9.406	29.698	33.615	1.00	62.19
4014	CA	GLU	755	9.040	31.101	33.535	1.00	60.87
4015	CB	GLU	755	8.481	31.550	34.891	1.00	60.79
4016	CG	GLU	755	7.821	32.911	34.858	1.00	62.93
4017	CD	GLU	755	6.333	32.829	35.097	1.00	56.10
4018	OE1	GLU	755	5.741	31.746	34.841	1.00	59.07
4019	OE2	GLU	755	5.761	33.857	35.531	1.00	65.63
4020	C	GLU	755	10.163	32.053	33.106	1.00	64.44
4021	O	GLU	755	10.006	33.269	33.209	1.00	61.31
4022	N	ILE	756	11.296	31.528	32.653	1.00	60.43
4023	CA	ILE	756	12.382	32.396	32.187	1.00	58.74

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	4024	CB	ILE	756	13.664	32.292	33.024	1.00	62.34
	4025	CG2	ILE	756	14.819	32.942	32.280	1.00	62.52
	4026	CG1	ILE	756	13.487	33.000	34.355	1.00	61.56
10	4027	CD1	ILE	756	14.750	33.012	35.170	1.00	59.91
	4028	C	ILE	756	12.725	31.933	30.799	1.00	61.14
	4029	O	ILE	756	12.985	32.732	29.904	1.00	61.35
15	4030	N	ILE	757	12.728	30.618	30.639	1.00	58.95
	4031	CA	ILE	757	13.026	30.016	29.362	1.00	60.81
	4032	CB	ILE	757	12.990	28.467	29.480	1.00	60.69
20	4033	CG2	ILE	757	12.522	27.838	28.197	1.00	64.94
	4034	CG1	ILE	757	14.378	27.948	29.883	1.00	60.19
	4035	CD1	ILE	757	14.463	27.436	31.313	1.00	62.89
25	4036	C	ILE	757	12.012	30.542	28.348	1.00	59.56
	4037	O	ILE	757	12.397	30.991	27.276	1.00	61.79
	4038	N	THR	758	10.726	30.521	28.702	1.00	61.66
30	4039	CA	THR	758	9.677	31.014	27.795	1.00	61.59
	4040	CB	THR	758	8.224	30.722	28.323	1.00	63.29
	4041	OG1	THR	758	8.188	30.811	29.755	1.00	62.91
35	4042	CG2	THR	758	7.754	29.343	27.874	1.00	61.73
	4043	C	THR	758	9.809	32.516	27.566	1.00	60.10
	4044	O	THR	758	9.735	33.002	26.423	1.00	59.44
40	4045	N	ASN	759	10.023	33.242	28.656	1.00	59.76
	4046	CA	ASN	759	10.154	34.691	28.608	1.00	61.77
	4047	CB	ASN	759	10.160	35.242	30.034	1.00	62.16
45	4048	CG	ASN	759	9.352	34.371	30.981	1.00	60.61
	4049	OD1	ASN	759	9.601	33.164	31.072	1.00	60.73
	4050	ND2	ASN	759	8.379	34.965	31.683	1.00	58.61
50	4051	C	ASN	759	11.430	35.091	27.886	1.00	63.83
	4052	O	ASN	759	11.725	36.278	27.737	1.00	59.18
	4053	N	GLN	760	12.191	34.099	27.439	1.00	60.77
55	4054	CA	GLN	760	13.431	34.395	26.742	1.00	60.74
	4055	CB	GLN	760	14.637	34.295	27.690	1.00	63.92
	4056	CG	GLN	760	14.546	35.101	28.992	1.00	63.35
	4057	CD	GLN	760	15.114	36.508	28.896	1.00	61.91
	4058	OE1	GLN	760	16.231	36.714	28.423	1.00	61.24
	4059	NE2	GLN	760	14.351	37.482	29.367	1.00	62.64
	4060	C	GLN	760	13.687	33.482	25.554	1.00	61.67

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM	
5	4061	O	GLN	760	14.390	33.898	24.631	1.00	58.73
	4062	N	ILE	761	13.124	32.264	25.563	1.00	63.30
	4063	CA	ILE	761	13.368	31.305	24.476	1.00	62.33
10	4064	CB	ILE	761	12.102	30.454	24.088	1.00	62.35
	4065	CG2	ILE	761	12.345	29.721	22.777	1.00	64.29
	4066	CG1	ILE	761	11.834	29.367	25.140	1.00	60.68
15	4067	CD1	ILE	761	12.794	28.186	25.074	1.00	65.98
	4068	C	ILE	761	13.925	32.069	23.273	1.00	60.92
	4069	O	ILE	761	15.089	31.875	22.912	1.00	60.54
20	4070	N	PRO	762	13.128	32.938	22.626	1.00	60.85
	4071	CD	PRO	762	11.810	32.652	22.044	1.00	60.12
	4072	CA	PRO	762	13.999	33.474	21.571	1.00	60.84
25	4073	CB	PRO	762	13.355	32.980	20.264	1.00	58.66
	4074	CG	PRO	762	12.240	32.017	20.716	1.00	58.17
	4075	C	PRO	762	14.222	34.968	21.533	1.00	62.93
30	4076	O	PRO	762	14.168	35.566	20.457	1.00	59.88
	4077	N	LYS	763	14.405	35.599	22.687	1.00	59.58
	4078	CA	LYS	763	14.750	37.015	22.653	1.00	62.56
35	4079	CB	LYS	763	14.713	37.645	24.045	1.00	61.84
	4080	CG	LYS	763	15.014	39.141	24.061	1.00	61.96
	4081	CD	LYS	763	14.703	39.723	25.430	1.00	62.42
40	4082	CE	LYS	763	13.428	39.096	25.979	1.00	61.00
	4083	NZ	LYS	763	12.992	39.651	27.285	1.00	62.85
	4084	C	LYS	763	16.182	36.666	22.292	1.00	58.43
45	4085	O	LYS	763	16.780	37.217	21.354	1.00	59.83
	4086	N	TYR	764	16.668	35.665	23.036	1.00	59.46
	4087	CA	TYR	764	17.999	35.106	22.895	1.00	61.50
50	4088	CB	TYR	764	18.291	34.109	24.020	1.00	62.35
	4089	CG	TYR	764	19.085	34.715	25.149	1.00	57.24
	4090	CD1	TYR	764	18.526	34.872	26.424	1.00	62.21
55	4091	CE1	TYR	764	19.236	35.509	27.451	1.00	63.69
	4092	CD2	TYR	764	20.378	35.200	24.927	1.00	62.73
	4093	CE2	TYR	764	21.095	35.837	25.942	1.00	62.44
55	4094	CZ	TYR	764	20.516	35.992	27.195	1.00	65.70
	4095	OH	TYR	764	21.206	36.670	28.168	1.00	63.44
	4096	C	TYR	764	18.156	34.400	21.570	1.00	60.32
	4097	O	TYR	764	17.580	34.816	20.556	1.00	60.80

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	4098	N	SER	765	18.922	33.310	21.597	1.00	62.63
	4099	CA	SER	765	19.209	32.535	20.391	1.00	62.57
	4100	CB	SER	765	17.908	31.971	19.777	1.00	63.02
10	4101	OG	SER	765	18.172	31.232	18.586	1.00	63.09
	4102	C	SER	765	19.904	33.487	19.403	1.00	61.20
	4103	O	SER	765	21.121	33.703	19.474	1.00	60.85
15	4104	N	ASN	766	19.099	34.064	18.513	1.00	59.31
	4105	CA	ASN	766	19.520	35.005	17.477	1.00	61.38
	4106	CB	ASN	766	18.344	35.932	17.155	1.00	63.73
20	4107	CG	ASN	766	17.006	35.195	17.116	1.00	60.04
	4108	OD1	ASN	766	16.493	34.720	18.153	1.00	64.69
	4109	ND2	ASN	766	16.433	35.091	15.916	1.00	59.73
25	4110	C	ASN	766	20.764	35.857	17.800	1.00	64.20
	4111	O	ASN	766	21.906	35.462	17.491	1.00	60.72
	4112	N	GLY	767	20.523	37.032	18.396	1.00	59.36
30	4113	CA	GLY	767	21.589	37.961	18.766	1.00	63.17
	4114	C	GLY	767	21.096	39.388	19.032	1.00	61.77
	4115	O	GLY	767	21.905	40.321	19.172	1.00	58.54
35	4116	N	ASN	768	19.772	39.550	19.118	1.00	61.70
	4117	CA	ASN	768	19.115	40.849	19.347	1.00	60.25
	4118	CB	ASN	768	17.603	40.673	19.163	1.00	61.86
40	4119	CG	ASN	768	17.257	39.882	17.898	1.00	63.48
	4120	OD1	ASN	768	17.602	38.702	17.772	1.00	58.87
	4121	ND2	ASN	768	16.579	40.534	16.956	1.00	59.56
45	4122	C	ASN	768	19.400	41.566	20.692	1.00	61.21
	4123	O	ASN	768	18.781	42.595	20.987	1.00	57.65
	4124	N	ILE	769	20.323	41.011	21.490	1.00	60.01
50	4125	CA	ILE	769	20.764	41.563	22.792	1.00	60.44
	4126	CB	ILE	769	20.851	40.456	23.891	1.00	60.23
	4127	CG2	ILE	769	21.520	41.004	25.161	1.00	65.73
55	4128	CG1	ILE	769	19.461	39.920	24.234	1.00	64.63
	4129	CD1	ILE	769	19.506	38.773	25.256	1.00	63.56
	4130	C	ILE	769	22.197	42.097	22.594	1.00	60.12
55	4131	O	ILE	769	22.744	41.990	21.495	1.00	59.38
	4132	N	LYS	770	22.799	42.660	23.643	1.00	58.87
	4133	CA	LYS	770	24.173	43.171	23.568	1.00	63.22
	4134	CB	LYS	770	24.210	44.693	23.711	1.00	61.35

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	4135	CG	LYS	770	25.615	45.304	23.656	1.00	60.38
	4136	CD	LYS	770	25.617	46.682	24.324	1.00	59.38
	4137	CE	LYS	770	26.765	47.580	23.858	1.00	63.47
10	4138	NZ	LYS	770	26.704	48.946	24.493	1.00	63.76
	4139	C	LYS	770	25.039	42.568	24.665	1.00	59.00
	4140	O	LYS	770	24.962	42.967	25.829	1.00	63.74
15	4141	N	LYS	771	25.868	41.604	24.292	1.00	59.72
	4142	CA	LYS	771	26.742	40.984	25.268	1.00	60.78
	4143	CB	LYS	771	27.024	39.525	24.871	1.00	59.33
20	4144	CG	LYS	771	27.854	39.345	23.619	1.00	62.03
	4145	CD	LYS	771	28.351	37.906	23.466	1.00	63.82
	4146	CE	LYS	771	29.538	37.838	22.501	1.00	59.76
25	4147	NZ	LYS	771	30.301	36.550	22.571	1.00	57.46
	4148	C	LYS	771	28.044	41.798	25.413	1.00	61.42
	4149	O	LYS	771	28.800	41.976	24.459	1.00	58.76
30	4150	N	LEU	772	28.271	42.302	26.623	1.00	61.95
	4151	CA	LEU	772	29.444	43.107	26.948	1.00	60.44
	4152	CB	LEU	772	29.187	43.864	28.260	1.00	59.38
35	4153	CG	LEU	772	27.923	44.730	28.267	1.00	63.13
	4154	CD1	LEU	772	27.630	45.253	29.656	1.00	60.11
	4155	CD2	LEU	772	28.102	45.873	27.289	1.00	62.17
40	4156	C	LEU	772	30.732	42.272	27.060	1.00	60.10
	4157	O	LEU	772	30.764	41.233	27.718	1.00	60.79
	4158	N	LEU	773	31.797	42.749	26.423	1.00	61.72
45	4159	CA	LEU	773	33.074	42.055	26.428	1.00	60.85
	4160	CB	LEU	773	33.406	41.580	25.011	1.00	62.82
	4161	CG	LEU	773	32.425	40.675	24.265	1.00	63.82
50	4162	CD1	LEU	773	32.927	40.451	22.866	1.00	60.94
	4163	CD2	LEU	773	32.285	39.352	24.966	1.00	62.11
	4164	C	LEU	773	34.205	42.942	26.933	1.00	63.04
55	4165	O	LEU	773	34.271	44.126	26.625	1.00	62.16
	4166	N	PHE	774	35.101	42.352	27.712	1.00	60.13
	4167	CA	PHE	774	36.246	43.072	28.248	1.00	61.57
	4168	CB	PHE	774	36.893	42.279	29.377	1.00	66.09
	4169	CG	PHE	774	36.280	42.543	30.698	1.00	61.67
	4170	CD1	PHE	774	36.524	43.741	31.355	1.00	59.42
	4171	CD2	PHE	774	35.385	41.650	31.248	1.00	56.29

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	4172	CE1	PHE	774	35.879	44.050	32.536	1.00	64.79
	4173	CE2	PHE	774	34.729	41.948	32.435	1.00	61.83
	4174	CZ	PHE	774	34.978	43.155	33.080	1.00	62.07
10	4175	C	PHE	774	37.243	43.261	27.143	1.00	58.09
	4176	O	PHE	774	38.081	44.155	27.187	1.00	63.24
	4177	N	HIS	775	37.131	42.398	26.143	1.00	61.71
15	4178	CA	HIS	775	38.022	42.419	25.007	1.00	60.58
	4179	CB	HIS	775	39.060	41.319	25.175	1.00	63.99
	4180	CG	HIS	775	39.763	41.365	26.492	1.00	62.38
20	4181	CD2	HIS	775	39.696	40.548	27.567	1.00	61.52
	4182	ND1	HIS	775	40.616	42.389	26.838	1.00	62.48
	4183	CE1	HIS	775	41.042	42.202	28.074	1.00	59.32
25	4184	NE2	HIS	775	40.498	41.092	28.538	1.00	62.24
	4185	C	HIS	775	37.236	42.196	23.732	1.00	61.77
	4186	O	HIS	775	36.461	41.252	23.633	1.00	62.62
30	4187	N	GLN	776	37.425	43.083	22.765	1.00	58.75
	4188	CA	GLN	776	36.759	42.955	21.484	1.00	58.47
	4189	CB	GLN	776	36.460	44.340	20.893	1.00	58.08
35	4190	CG	GLN	776	37.681	45.247	20.680	1.00	63.95
	4191	CD	GLN	776	38.236	45.221	19.250	1.00	62.81
	4192	OE1	GLN	776	39.158	45.979	18.924	1.00	62.48
40	4193	NE2	GLN	776	37.680	44.353	18.397	1.00	60.08
	4194	C	GLN	776	37.724	42.163	20.599	1.00	60.33
	4195	O	GLN	776	37.269	41.235	19.894	1.00	61.93
45	4196	OXT	GLN	776	38.936	42.474	20.642	1.00	63.26
	4197	CB	LYS	741	7.500	39.003	28.905	1.00	62.43
	4198	CG	LYS	741	8.600	39.530	28.004	1.00	60.91
50	4199	CD	LYS	741	9.141	40.875	28.431	1.00	59.52
	4200	CE	LYS	741	10.182	41.314	27.418	1.00	62.38
	4201	NZ	LYS	741	10.807	42.617	27.779	1.00	64.43
55	4202	C	LYS	741	6.303	36.975	29.773	1.00	61.31
	4203	O	LYS	741	6.054	35.766	29.829	1.00	59.09
	4204	N	LYS	741	6.417	37.458	27.272	1.00	62.30
55	4205	CA	LYS	741	7.109	37.544	28.597	1.00	59.65
	4206	N	GLU	742	5.905	37.867	30.689	1.00	62.69
	4207	CA	GLU	742	5.163	37.547	31.917	1.00	61.65
	4208	CB	GLU	742	4.672	36.083	31.926	1.00	61.06

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	4209	CG	GLU	742	4.087	35.564	33.257	1.00	61.09
	4210	CD	GLU	742	2.705	36.123	33.568	1.00	62.31
	4211	OE1	GLU	742	2.138	35.720	34.616	1.00	57.45
10	4212	OE2	GLU	742	2.195	36.960	32.771	1.00	60.87
	4213	C	GLU	742	6.112	37.794	33.099	1.00	63.06
	4214	O	GLU	742	5.915	38.741	33.853	1.00	61.76
15	4215	N	ASN	743	7.151	36.967	33.238	1.00	63.03
	4216	CA	ASN	743	8.116	37.101	34.341	1.00	61.82
	4217	CB	ASN	743	9.276	38.040	33.958	1.00	58.35
20	4218	CG	ASN	743	10.217	37.445	32.909	1.00	59.24
	4219	OD1	ASN	743	10.071	37.693	31.699	1.00	60.28
	4220	ND2	ASN	743	11.198	36.658	33.372	1.00	60.70
25	4221	C	ASN	743	7.447	37.656	35.604	1.00	61.37
	4222	O	ASN	743	8.010	38.522	36.284	1.00	60.15
	4223	N	ALA	744	6.245	37.167	35.907	1.00	60.68
30	4224	CA	ALA	744	5.497	37.626	37.073	1.00	62.31
	4225	CB	ALA	744	4.024	37.229	36.940	1.00	62.38
	4226	C	ALA	744	6.080	37.067	38.364	1.00	61.35
35	4227	O	ALA	744	6.168	37.778	39.360	1.00	59.70
	4228	N	LEU	745	6.490	35.801	38.346	1.00	61.20
	4229	CA	LEU	745	7.062	35.182	39.538	1.00	59.93
40	4230	CB	LEU	745	7.419	33.710	39.276	1.00	63.15
	4231	CG	LEU	745	7.255	32.720	40.448	1.00	63.24
	4232	CD1	LEU	745	8.022	31.429	40.158	1.00	59.45
45	4233	CD2	LEU	745	7.759	33.342	41.745	1.00	59.90
	4234	C	LEU	745	8.313	35.934	39.987	1.00	59.41
	4235	O	LEU	745	8.520	36.123	41.182	1.00	59.83
50	4236	N	LEU	746	9.137	36.372	39.031	1.00	63.44
	4237	CA	LEU	746	10.375	37.096	39.350	1.00	60.90
	4238	CB	LEU	746	11.266	37.239	38.104	1.00	63.43
55	4239	CG	LEU	746	12.771	36.991	38.300	1.00	64.10
	4240	CD1	LEU	746	13.540	37.598	37.140	1.00	61.93
	4241	CD2	LEU	746	13.248	37.598	39.612	1.00	58.02
	4242	C	LEU	746	10.120	38.485	39.950	1.00	65.26
	4243	O	LEU	746	10.649	38.808	41.025	1.00	59.76
	4244	N	ARG	747	9.334	39.308	39.255	1.00	61.19
	4245	CA	ARG	747	9.012	40.641	39.762	1.00	61.73

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	4246	CB	ARG	747	7.844	41.256	38.975	1.00	59.04
	4247	CG	ARG	747	7.475	42.676	39.421	1.00	57.13
	4248	CD	ARG	747	6.596	43.434	38.407	1.00	58.93
10	4249	NE	ARG	747	7.362	44.324	37.522	1.00	59.01
	4250	CZ	ARG	747	7.556	44.118	36.221	1.00	59.60
	4251	NH1	ARG	747	7.039	43.043	35.624	1.00	63.96
15	4252	NH2	ARG	747	8.272	44.987	35.518	1.00	60.37
	4253	C	ARG	747	8.651	40.511	41.247	1.00	61.37
	4254	O	ARG	747	9.155	41.257	42.090	1.00	62.28
20	4255	N	TYR	748	7.799	39.541	41.565	1.00	62.06
	4256	CA	TYR	748	7.399	39.306	42.941	1.00	60.54
	4257	CB	TYR	748	6.517	38.050	43.003	1.00	60.69
25	4258	CG	TYR	748	6.287	37.521	44.401	1.00	59.67
	4259	CD1	TYR	748	7.077	36.488	44.908	1.00	60.21
	4260	CE1	TYR	748	6.926	36.044	46.209	1.00	60.77
30	4261	CD2	TYR	748	5.329	38.093	45.240	1.00	63.30
	4262	CE2	TYR	748	5.174	37.654	46.550	1.00	61.08
	4263	CZ	TYR	748	5.977	36.631	47.027	1.00	62.49
35	4264	OH	TYR	748	5.864	36.204	48.331	1.00	59.76
	4265	C	TYR	748	8.593	39.190	43.908	1.00	63.27
	4266	O	TYR	748	8.702	39.969	44.857	1.00	60.19
40	4267	N	LEU	749	9.484	38.229	43.663	1.00	62.27
	4268	CA	LEU	749	10.661	38.008	44.516	1.00	62.12
	4269	CB	LEU	749	11.454	36.792	44.020	1.00	64.20
45	4270	CG	LEU	749	10.690	35.476	43.873	1.00	58.72
	4271	CD1	LEU	749	11.058	34.828	42.554	1.00	61.26
	4272	CD2	LEU	749	10.986	34.565	45.039	1.00	61.68
50	4273	C	LEU	749	11.589	39.223	44.561	1.00	61.27
	4274	O	LEU	749	12.241	39.497	45.571	1.00	60.09
	4275	N	LEU	750	11.658	39.946	43.455	1.00	60.39
55	4276	CA	LEU	750	12.503	41.120	43.397	1.00	59.95
	4277	CB	LEU	750	12.603	41.607	41.959	1.00	59.67
	4278	CG	LEU	750	14.026	41.742	41.404	1.00	65.62
55	4279	CD1	LEU	750	15.031	40.919	42.205	1.00	61.72
	4280	CD2	LEU	750	14.005	41.302	39.953	1.00	61.66
	4281	C	LEU	750	11.954	42.216	44.298	1.00	58.16
	4282	O	LEU	750	12.712	42.855	45.032	1.00	61.93

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
4283	N	ASP	751	10.637	42.423	44.242	1.00	60.02
4284	CA	ASP	751	9.969	43.428	45.073	1.00	61.63
4285	CB	ASP	751	8.539	43.658	44.616	1.00	59.82
4286	CG	ASP	751	8.381	44.973	43.912	1.00	60.49
4287	OD1	ASP	751	9.166	45.214	42.968	1.00	59.40
4288	OD2	ASP	751	7.491	45.767	44.298	1.00	59.17
4289	C	ASP	751	9.941	43.037	46.531	1.00	62.48
4290	O	ASP	751	10.367	43.813	47.383	1.00	63.09
4291	N	LYS	752	9.421	41.841	46.808	1.00	64.09
4292	CA	LYS	752	9.346	41.308	48.164	1.00	60.89
4293	CB	LYS	752	9.881	39.882	48.216	1.00	63.21
4294	CG	LYS	752	9.051	38.811	47.568	1.00	57.72
4295	CD	LYS	752	9.168	37.532	48.396	1.00	60.58
4296	CE	LYS	752	8.769	37.801	49.858	1.00	63.26
4297	NZ	LYS	752	8.598	36.571	50.686	1.00	60.07
4298	C	LYS	752	10.218	42.123	49.090	1.00	59.75
4299	O	LYS	752	11.426	42.228	48.869	1.00	61.26
4300	N	ASP	753	9.644	42.700	50.132	1.00	64.75
4301	CA	ASP	753	10.478	43.462	51.039	1.00	60.32
4302	CB	ASP	753	9.643	44.126	52.126	1.00	62.72
4303	CG	ASP	753	10.496	44.762	53.198	1.00	62.87
4304	OD1	ASP	753	11.420	45.549	52.863	1.00	59.14
4305	OD2	ASP	753	10.239	44.468	54.382	1.00	63.19
4306	C	ASP	753	11.455	42.468	51.647	1.00	60.33
4307	O	ASP	753	12.111	42.750	52.646	1.00	61.12
4308	N	ALA	754	11.528	41.304	51.008	1.00	59.93
4309	CA	ALA	754	12.396	40.177	51.356	1.00	61.16
4310	CB	ALA	754	12.896	39.509	50.053	1.00	64.36
4311	C	ALA	754	13.587	40.401	52.307	1.00	59.44
4312	O	ALA	754	14.700	39.937	52.047	1.00	61.71
4313	N	THR	755	13.355	41.108	53.403	1.00	60.67
4314	CA	THR	755	14.375	41.342	54.420	1.00	60.98
4315	CB	THR	755	15.250	42.613	54.137	1.00	63.96
4316	OG1	THR	755	14.460	43.794	54.313	1.00	60.28
4317	CG2	THR	755	15.824	42.582	52.696	1.00	57.43
4318	C	THR	755	13.505	41.499	55.671	1.00	59.27
4319	O	THR	755	13.323	42.586	56.237	1.00	60.51

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	4320	N	ALA	756	12.918	40.356	56.024	1.00	62.21
	4321	CA	ALA	756	12.025	40.165	57.162	1.00	59.83
	4322	CB	ALA	756	11.075	38.993	56.870	1.00	60.21
10	4323	C	ALA	756	12.890	39.842	58.372	1.00	61.08
	4324	O	ALA	756	12.461	39.941	59.531	1.00	61.80
	4325	N	ALA	757	14.115	39.426	58.072	1.00	62.43
15	4326	CA	ALA	757	15.087	39.099	59.092	1.00	60.57
	4327	CB	ALA	757	16.415	38.753	58.431	1.00	60.81
	4328	C	ALA	757	15.211	40.367	59.932	1.00	61.35
20	4329	O	ALA	757	15.146	41.460	59.327	1.00	62.10
	4330	OXT	ALA	757	15.354	40.253	61.169	1.00	58.48
	4331	O	HOH	1	62.349	-1.370	59.183	1.00	61.82
25	4332	O	HOH	2	63.098	9.775	56.010	1.00	63.21
	4333	O	HOH	3	29.467	50.468	47.493	1.00	60.82
	4334	O	HOH	4	24.799	1.025	51.054	1.00	63.04
30	4335	O	HOH	5	25.120	35.371	29.890	1.00	58.53
	4336	O	HOH	6	62.603	13.819	69.179	1.00	62.10
	4337	O	HOH	7	43.394	-0.575	64.086	1.00	61.07
35	4338	O	HOH	8	33.029	27.080	24.812	1.00	63.53
	4339	O	HOH	9	40.476	0.604	50.517	1.00	62.87
	4340	O	HOH	10	42.083	33.017	29.431	1.00	59.31
40	4341	O	HOH	11	40.224	-1.905	63.310	1.00	60.38
	4342	O	HOH	12	29.926	49.219	30.317	1.00	60.19
	4343	O	HOH	13	63.481	3.211	57.703	1.00	62.93
45	4344	O	HOH	14	45.679	44.833	38.756	1.00	60.97
	4345	O	HOH	15	21.388	1.839	41.400	1.00	61.41
	4346	O	HOH	16	47.452 -	16.061	63.707	1.00	60.73
50	4347	O	HOH	17	52.653	15.955	63.901	1.00	64.75
	4348	O	HOH	18	62.913	1.964	67.923	1.00	64.33
	4349	O	HOH	19	62.507	3.936	69.792	1.00	60.95
55	4350	O	HOH	20	11.730	26.749	44.436	1.00	60.79
	4351	O	HOH	21	48.735	13.308	64.587	1.00	62.06
	4352	O	HOH	22	32.377	39.863	58.144	1.00	63.51
55	4353	O	HOH	23	58.924	9.831	70.947	1.00	61.40
	4354	O	HOH	24	39.278	17.448	64.290	1.00	62.12
	4355	O	HOH	25	40.573	48.042	36.816	1.00	60.96
	4356	O	HOH	26	40.494	35.299	48.387	1.00	59.93

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
4357	O	HOH	27	61.454	1.678	61.901	1.00	60.51
4358	O	HOH	28	9.075	22.638	42.296	1.00	61.65
4359	O	HOH	29	51.369	13.900	63.592	1.00	64.00
4360	O	HOH	30	61.184	-0.481	44.937	1.00	61.95
4361	O	HOH	31	19.041	16.035	52.737	1.00	60.85
4362	O	HOH	32	37.487	3.963	49.092	1.00	60.40
4363	O	HOH	33	31.183	34.399	55.395	1.00	61.32
4364	O	HOH	34	25.672	33.490	53.795	1.00	61.76
4365	O	HOH	35	24.467	27.177	45.107	1.00	62.37
4366	O	HOH	36	47.899	30.685	35.691	1.00	60.62
4367	O	HOH	37	31.250	45.014	24.427	1.00	63.26
4368	O	HOH	38	60.719	-0.340	49.987	1.00	60.94
4369	O	HOH	39	48.761	14.305	46.147	1.00	59.45
4370	O	HOH	40	52.252	11.824	45.533	1.00	59.86
4371	O	HOH	41	40.704	30.604	47.765	1.00	62.04
4372	O	HOH	42	34.599	19.541	73.265	1.00	61.69
4373	O	HOH	43	44.135	32.951	48.092	1.00	60.11
4374	O	HOH	44	16.447	16.136	55.224	1.00	58.77
4375	O	HOH	45	37.470	21.079	29.057	1.00	61.47
4376	O	HOH	46	14.411	15.785	52.085	1.00	58.97
4377	O	HOH	47	27.199	25.588	51.919	1.00	58.58
4378	O	HOH	48	32.466	25.097	53.254	1.00	60.88
4379	O	HOH	49	17.927	39.612	49.972	1.00	61.48
4380	O	HOH	50	17.243	38.022	52.339	1.00	61.61
4381	O	HOH	51	65.714	6.374	72.458	1.00	61.45
4382	O	HOH	52	25.540	34.686	57.601	1.00	59.81
4383	O	HOH	53	22.812	3.452	38.767	1.00	62.42
4384	C1	DEX	1	31.791	3.330	56.615	1.00	59.00
4385	H1	DEX	1	30.892	2.719	56.626	1.00	59.00
4386	C2	DEX	1	32.066	4.057	55.552	1.00	59.00
4387	H2	DEX	1	31.418	4.016	54.717	1.00	59.00
4388	C3	DEX	1	33.314	4.929	55.514	1.00	59.00
4389	C4	DEX	1	34.176	5.061	56.733	1.00	59.00
4390	H4	DEX	1	35.013	5.729	56.720	1.00	59.00
4391	C5	DEX	1	33.915	4.329	57.855	1.00	59.00
4392	C6	DEX	1	34.782	4.456	59.133	1.00	59.00
4393	H61	DEX	1	35.558	5.172	59.015	1.00	59.00

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TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
5	4394	H62	DEX	1	35.262	3.483	59.339	1.00	59.00
	4395	C7	DEX	1	33.905	4.834	60.331	1.00	59.00
	4396	H71	DEX	1	33.520	5.861	60.202	1.00	59.00
10	4397	H72	DEX	1	34.515	4.837	61.236	1.00	59.00
	4398	C8	DEX	1	32.690	3.903	60.544	1.00	59.00
	4399	H8	DEX	1	33.063	2.878	60.787	1.00	59.00
15	4400	C9	DEX	1	31.759	3.803	59.162	1.00	59.00
	4401	C10	DEX	1	32.677	3.304	57.900	1.00	59.00
	4402	C11	DEX	1	30.360	2.986	59.327	1.00	59.00
20	4403	H11	DEX	1	29.743	3.203	58.478	1.00	59.00
	4404	C12	DEX	1	29.599	3.415	60.596	1.00	59.00
	4405	H121	DEX	1	28.744	2.788	60.729	1.00	59.00
25	4406	H122	DEX	1	29.221	4.448	60.436	1.00	59.00
	4407	C13	DEX	1	30.518	3.414	61.924	1.00	59.00
	4408	C14	DEX	1	31.758	4.387	61.726	1.00	59.00
30	4409	H14	DEX	1	31.359	5.403	61.401	1.00	59.00
	4410	C15	DEX	1	32.374	4.589	63.095	1.00	59.00
	4411	H151	DEX	1	32.893	5.547	63.111	1.00	59.00
35	4412	H152	DEX	1	33.119	3.796	63.281	1.00	59.00
	4413	C16	DEX	1	31.175	4.486	64.093	1.00	59.00
	4414	H16	DEX	1	31.391	3.605	64.743	1.00	59.00
40	4415	C17	DEX	1	29.863	4.144	63.168	1.00	59.00
	4416	C18	DEX	1	30.929	1.834	62.325	1.00	59.00
	4417	H181	DEX	1	31.535	1.833	63.241	1.00	59.00
45	4418	H182	DEX	1	30.050	1.248	62.496	1.00	59.00
	4419	H183	DEX	1	31.537	1.374	61.558	1.00	59.00
	4420	C19	DEX	1	33.270	1.833	58.015	1.00	59.00
50	4421	H191	DEX	1	33.916	1.724	58.905	1.00	59.00
	4422	H192	DEX	1	32.485	1.095	58.112	1.00	59.00
	4423	H193	DEX	1	33.870	1.605	57.134	1.00	59.00
55	4424	C20	DEX	1	28.759	3.270	63.873	1.00	59.00
	4425	C21	DEX	1	27.338	3.348	63.353	1.00	59.00
	4426	H211	DEX	1	27.350	3.637	62.283	1.00	59.00
	4427	H212	DEX	1	26.827	4.148	63.876	1.00	59.00
	4428	C22	DEX	1	31.008	5.693	64.947	1.00	59.00
	4429	H221	DEX	1	30.160	5.560	65.619	1.00	59.00
	4430	H222	DEX	1	31.912	5.877	65.542	1.00	59.00

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
4431	H223	DEX	1	30.811	6.588	64.313	1.00	59.00
4432	F1	DEX	1	31.331	5.130	58.833	1.00	59.00
4433	O1	DEX	1	33.617	5.512	54.507	1.00	59.00
4434	O2	DEX	1	30.601	1.580	59.361	1.00	59.00
4435	HO2	DEX	1	29.784	1.163	59.706	1.00	59.00
4436	O3	DEX	1	29.236	5.409	62.711	1.00	59.00
4437	H3	DEX	1	28.816	5.780	63.475	1.00	59.00
4438	O4	DEX	1	29.058	2.511	64.818	1.00	59.00
4439	O5	DEX	1	26.689	2.117	63.492	1.00	59.00
4440	H5	DEX	1	25.816	2.344	63.756	1.00	59.00
4441	C1	DEX	1	21.344	23.582	37.624	1.00	59.00
4442	H1	DEX	1	20.325	23.208	37.634	1.00	59.00
4443	C2	DEX	1	22.105	23.392	38.670	1.00	59.00
4444	H2	DEX	1	21.710	22.910	39.509	1.00	59.00
4445	C3	DEX	1	23.539	23.892	38.687	1.00	59.00
4446	C4	DEX	1	24.137	24.501	37.450	1.00	59.00
4447	H4	DEX	1	25.173	24.791	37.441	1.00	59.00
4448	C5	DEX	1	23.372	24.700	36.346	1.00	59.00
4449	C6	DEX	1	23.965	25.312	35.061	1.00	59.00
4450	H61	DEX	1	24.996	25.542	35.157	1.00	59.00
4451	H62	DEX	1	23.444	26.267	34.853	1.00	59.00
4452	C7	DEX	1	23.752	24.345	33.877	1.00	59.00
4453	H71	DEX	1	24.370	23.444	34.001	1.00	59.00
4454	H72	DEX	1	24.092	24.829	32.956	1.00	59.00
4455	C8	DEX	1	22.275	23.885	33.692	1.00	59.00
4456	H8	DEX	1	21.638	24.764	33.460	1.00	59.00
4457	C9	DEX	1	21.676	23.232	35.081	1.00	59.00
4458	C10	DEX	1	21.819	24.294	36.329	1.00	59.00
4459	C11	DEX	1	20.197	22.585	34.938	1.00	59.00
4460	H11	DEX	1	20.028	21.974	35.784	1.00	59.00
4461	C12	DEX	1	20.107	21.699	33.700	1.00	59.00
4462	H121	DEX	1	19.130	21.365	33.602	1.00	59.00
4463	H122	DEX	1	20.720	20.795	33.859	1.00	59.00
4464	C13	DEX	1	20.600	22.429	32.344	1.00	59.00
4465	C14	DEX	1	22.105	22.863	32.515	1.00	59.00
4466	H14	DEX	1	22.701	21.953	32.834	1.00	59.00
4467	C15	DEX	1	22.602	23.242	31.129	1.00	59.00

TABLE 3 (continued)

ATOMIC COORDINATES FOR THE GR/TIF2/DEX MODEL USED IN MOLECULAR REPLACEMENT								
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	B	ATOM
4468	H151	DEX	1	23.685	23.110	31.097	1.00	59.00
4469	H152	DEX	1	22.383	24.310	30.934	1.00	59.00
4470	C16	DEX	1	21.806	22.306	30.152	1.00	59.00
4471	H16	DEX	1	21.207	22.984	29.504	1.00	59.00
4472	C17	DEX	1	20.783	21.450	31.097	1.00	59.00
4473	C18	DEX	1	19.540	23.677	31.944	1.00	59.00
4474	H181	DEX	1	19.873	24.157	31.015	1.00	59.00
4475	H182	DEX	1	18.547	23.297	31.792	1.00	59.00
4476	H183	DEX	1	19.525	24.449	32.700	1.00	59.00
4477	C19	DEX	1	20.959	25.638	36.205	1.00	59.00
4478	H191	DEX	1	21.232	26.215	35.303	1.00	59.00
4479	H192	DEX	1	19.899	25.426	36.127	1.00	59.00
4480	H193	DEX	1	21.132	26.270	37.072	1.00	59.00
4481	C20	DEX	1	19.417	21.067	30.421	1.00	59.00
4482	C21	DEX	1	18.443	20.176	31.204	1.00	59.00
4483	H211	DEX	1	17.932	20.800	31.959	1.00	59.00
4484	H212	DEX	1	19.031	19.423	31.779	1.00	59.00
4485	C22	DEX	1	22.671	21.454	29.301	1.00	59.00
4486	H221	DEX	1	22.061	20.835	28.644	1.00	59.00
4487	H222	DEX	1	23.334	22.077	28.688	1.00	59.00
4488	H223	DEX	1	23.300	20.785	29.933	1.00	59.00
4489	F1	DEX	1	22.519	22.128	35.397	1.00	59.00
4490	O	DEX	1	24.201	23.808	39.692	1.00	59.00
4491	O2	DEX	1	19.179	23.598	34.905	1.00	59.00
4492	HO2	DEX	1	18.367	23.168	34.580	1.00	59.00
4493	O3	DEX	1	21.444	20.210	31.554	1.00	59.00
4494	H3	DEX	1	21.502	19.648	30.802	1.00	59.00
4495	O4	DEX	1	19.127	21.505	29.299	1.00	59.00
4496	O5	DEX	1	17.530	19.572	30.381	1.00	59.00
4497	H5	DEX	1	17.435	18.711	30.744	1.00	59.00

TABLE 4

ATOMIC COORDINATES OF AR IN COMPLEX WITH BICALUTAMIDE
OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL
STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP

Atom Number	Atom Type	Residue Name	Residue Number	X Coordinate	Y Coordinate	Z Coordinate
1	N	ILE	672	-7.802	44.333	21.810
2	HN1	ILE	672	-8.615	43.811	21.453
3	HN2	ILE	672	-8.089	44.905	22.617
4	HN3	ILE	672	-7.435	44.946	21.068
5	CA	ILE	672	-6.772	43.402	22.220
6	C	ILE	672	-5.691	44.331	22.701
7	O	ILE	672	-5.692	45.515	22.363
8	CB	ILE	672	-6.276	42.491	21.024
9	CG1	ILE	672	-5.637	43.272	19.831
10	CG2	ILE	672	-7.403	41.575	20.455
11	CD1	ILE	672	-4.861	42.419	18.807
12	N	PHE	673	-4.769	43.820	23.494
13	CA	PHE	673	-3.723	44.678	24.008
14	HN	PHE	673	-4.793	42.850	23.738
15	C	PHE	673	-2.862	45.295	22.900
16	O	PHE	673	-2.512	46.478	22.951
17	CB	PHE	673	-2.800	43.874	24.973
18	CG	PHE	673	-1.802	44.693	25.806
19	CD1	PHE	673	-2.082	46.032	26.100
20	CE1	PHE	673	-1.154	46.810	26.784
21	CZ	PHE	673	0.054	46.249	27.194
22	CE2	PHE	673	0.335	44.913	26.915
23	CD2	PHE	673	-0.590	44.136	26.221
24	N	LEU	674	-2.522	44.494	21.898
25	CA	LEU	674	-1.722	44.978	20.786
26	HN	LEU	674	-2.821	43.540	21.909
27	C	LEU	674	-2.622	45.837	19.898
28	O	LEU	674	-2.149	46.600	19.056
29	CB	LEU	674	-1.153	43.767	19.994
30	CG	LEU	674	-2.157	42.828	19.272
31	CD1	LEU	674	-1.413	41.640	18.646
32	CD2	LEU	674	-3.264	42.312	20.205
33	N	ASN	675	-3.931	45.693	20.088
34	CA	ASN	675	-4.913	46.442	19.306
35	HN	ASN	675	-4.252	45.054	20.786
36	C	ASN	675	-4.860	47.910	19.668
37	O	ASN	675	-4.889	48.806	18.829
38	CB	ASN	675	-6.326	45.855	19.591
39	CG	ASN	675	-7.519	46.577	18.957
40	OD1	ASN	675	-8.064	46.168	17.942
41	ND2	ASN	675	-7.952	47.679	19.507
42	1HD2	ASN	675	-8.644	48.159	18.925
43	2HD2	ASN	675	-7.420	48.042	20.298
44	N	VAL	676	-4.799	48.126	20.963
45	CA	VAL	676	-4.752	49.439	21.528
46	HN	VAL	676	-4.785	47.339	21.580
47	C	VAL	676	-3.362	50.002	21.308

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48	O	VAL	676	-3.176	51.208	21.154
49	CB	VAL	676	-5.057	49.282	23.071
50	CG1	VAL	676	-5.366	50.591	23.849
51	CG2	VAL	676	-6.239	48.333	23.383
52	N	LEU	677	-2.374	49.119	21.292
53	CA	LEU	677	-1.001	49.552	21.090
54	HN	LEU	677	-2.574	48.147	21.419
55	C	LEU	677	-0.869	50.119	19.665
56	O	LEU	677	-0.131	51.073	19.421
57	CB	LEU	677	-0.068	48.363	21.316
58	CG	LEU	677	1.249	48.527	22.075
59	CD1	LEU	677	1.094	49.268	23.390
60	CD2	LEU	677	1.764	47.137	22.328
61	N	GLU	678	-1.606	49.544	18.727
62	CA	GLU	678	-1.548	50.045	17.376
63	HN	GLU	678	-2.197	48.770	18.954
64	C	GLU	678	-2.330	51.346	17.200
65	O	GLU	678	-1.845	52.246	16.524
66	CB	GLU	678	-2.055	49.004	16.399
67	CG	GLU	678	-2.187	49.525	14.999
68	CD	GLU	678	-2.559	48.425	14.030
69	OE1	GLU	678	-2.750	48.734	12.830
70	OE2	GLU	678	-2.654	47.252	14.473
71	HE2	GLU	678	-2.890	46.667	13.769
72	N	ALA	679	-3.518	51.484	17.797
73	CA	ALA	679	-4.251	52.738	17.584
74	HN	ALA	679	-3.895	50.756	18.370
75	C	ALA	679	-3.645	53.964	18.253
76	O	ALA	679	-4.043	55.082	17.931
77	CB	ALA	679	-5.746	52.562	17.903
78	N	ILE	680	-2.694	53.786	19.173
79	CA	ILE	680	-2.079	54.944	19.831
80	HN	ILE	680	-2.401	52.861	19.414
81	C	ILE	680	-0.672	55.231	19.325
82	O	ILE	680	0.069	56.001	19.939
83	CB	ILE	680	-1.980	54.783	21.367
84	CG2	ILE	680	-3.269	54.216	21.925
85	CG1	ILE	680	-0.801	53.879	21.725
86	CD1	ILE	680	-0.571	53.751	23.208
87	N	GLU	681	-0.301	54.606	18.214
88	CA	GLU	681	1.020	54.801	17.640
89	HN	GLU	681	-0.944	53.988	17.762
90	C	GLU	681	1.093	56.227	17.144
91	O	GLU	681	0.147	56.718	16.543
92	CB	GLU	681	1.237	53.825	16.483
93	CG	GLU	681	2.643	53.807	15.879
94	CD	GLU	681	3.760	53.831	16.920
95	OE1	GLU	681	3.570	53.258	18.018
96	OE2	GLU	681	4.832	54.412	16.631
97	HE2	GLU	681	5.431	54.351	17.360
98	N	PRO	682	2.175	56.936	17.458
99	CA	PRO	682	2.103	58.288	16.900
100	CD	PRO	682	2.934	56.915	18.715
101	C	PRO	682	2.205	58.244	15.379
102	O	PRO	682	2.532	57.209	14.789

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103	CB	PRO	682	3.278	59.025	17.552
104	CG	PRO	682	3.904	58.034	18.527
105	N	GLY	683	1.908	59.358	14.734
106	CA	GLY	683	1.978	59.373	13.291
107	HN	GLY	683	1.640	60.179	15.237
108	C	GLY	683	3.198	60.165	12.862
109	O	GLY	683	3.578	61.122	13.536
110	N	VAL	684	3.807	59.769	11.747
111	CA	VAL	684	5.011	60.440	11.267
112	HN	VAL	684	3.433	58.999	11.229
113	C	VAL	684	4.883	61.937	11.156
114	O	VAL	684	3.915	62.458	10.610
115	CB	VAL	684	5.466	59.926	9.887
116	CG1	VAL	684	5.969	58.504	10.001
117	CG2	VAL	684	4.322	60.031	8.885
118	N	VAL	685	5.876	62.639	11.673
119	CA	VAL	685	5.853	64.080	11.590
120	HN	VAL	685	6.640	62.174	12.120
121	C	VAL	685	7.097	64.568	10.856
122	O	VAL	685	8.225	64.160	11.169
123	CB	VAL	685	5.760	64.727	13.029
124	CG1	VAL	685	6.902	64.371	14.020
125	CG2	VAL	685	5.694	66.273	13.019
126	N	CYS	686	6.859	65.427	9.863
127	CA	CYS	686	7.899	65.995	9.007
128	HN	CYS	686	5.911	65.698	9.695
129	C	CYS	686	8.844	66.938	9.690
130	O	CYS	686	8.559	67.480	10.759
131	CB	CYS	686	7.230	66.625	7.770
132	SG	CYS	686	6.474	65.353	6.733
133	HG	CYS	686	7.391	65.368	5.769
134	N	ALA	687	9.970	67.152	9.023
135	CA	ALA	687	11.028	67.995	9.539
136	HN	ALA	687	10.094	66.714	8.133
137	C	ALA	687	10.956	69.476	9.185
138	O	ALA	687	11.644	70.281	9.806
139	CB	ALA	687	12.359	67.437	9.100
140	N	GLY	688	10.141	69.846	8.202
141	CA	GLY	688	10.070	71.249	7.828
142	HN	GLY	688	9.583	69.167	7.725
143	C	GLY	688	11.444	71.762	7.423
144	O	GLY	688	11.889	72.816	7.879
145	N	HIS	689	12.131	71.003	6.571
146	CA	HIS	689	13.464	71.376	6.102
147	HN	HIS	689	11.722	70.152	6.241
148	C	HIS	689	13.342	72.135	4.797
149	O	HIS	689	12.377	71.977	4.040
150	CB	HIS	689	14.316	70.110	5.908
151	CG	HIS	689	15.770	70.426	5.713
152	ND1	HIS	689	16.648	70.861	6.702
153	CE1	HIS	689	17.810	70.790	6.025
154	NE2	HIS	689	17.774	70.371	4.731
155	CD2	HIS	689	16.438	70.133	4.533
156	HE2	HIS	689	18.550	70.256	4.064
157	N	ASP	690	14.333	72.973	4.559

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158	CA	ASP	690	14.410	73.739	3.341
159	HN	ASP	690	15.053	73.080	5.244
160	C	ASP	690	15.539	73.046	2.609
161	O	ASP	690	16.711	73.253	2.928
162	CB	ASP	690	14.800	75.178	3.628
163	CG	ASP	690	14.786	76.022	2.386
164	OD1	ASP	690	14.680	75.431	1.294
165	OD2	ASP	690	14.880	77.259	2.497
166	HD2	ASP	690	14.857	77.655	1.640
167	N	ASN	691	15.183	72.196	1.658
168	CA	ASN	691	16.168	71.457	0.886
169	HN	ASN	691	14.211	72.058	1.467
170	C	ASN	691	16.414	72.208	-0.411
171	O	ASN	691	17.014	71.684	-1.351
172	CB	ASN	691	15.643	70.020	0.600
173	CG	ASN	691	14.332	69.904	-0.185
174	OD1	ASN	691	14.308	69.649	-1.380
175	ND2	ASN	691	13.204	70.107	0.441
176	1HD2	ASN	691	12.406	70.157	-0.199
177	2HD2	ASN	691	13.262	70.406	1.415
178	N	ASN	692	15.935	73.449	-0.435
179	CA	ASN	692	16.057	74.325	-1.592
180	HN	ASN	692	15.470	73.797	0.379
181	C	ASN	692	17.406	74.995	-1.581
182	O	ASN	692	17.708	75.846	-2.418
183	CB	ASN	692	14.916	75.383	-1.546
184	CG	ASN	692	15.214	76.694	-0.812
185	OD1	ASN	692	15.510	77.721	-1.406
186	ND2	ASN	692	15.173	76.709	0.493
187	1HD2	ASN	692	15.534	77.583	0.885
188	2HD2	ASN	692	15.013	75.817	0.961
189	N	GLN	693	18.223	74.651	-0.605
190	CA	GLN	693	19.516	75.267	-0.548
191	HN	GLN	693	17.947	73.976	0.079
192	C	GLN	693	20.441	74.218	0.032
193	O	GLN	693	20.051	73.480	0.945
194	CB	GLN	693	19.445	76.508	0.368
195	CG	GLN	693	18.110	77.323	0.324
196	CD	GLN	693	17.987	78.603	1.161
197	OE1	GLN	693	16.977	79.287	1.123
198	NE2	GLN	693	18.986	78.991	1.913
199	2HE2	GLN	693	19.825	78.413	1.846
200	1HE2	GLN	693	18.847	79.886	2.386
201	N	PRO	694	21.688	74.161	-0.473
202	CA	PRO	694	22.654	73.163	-0.016
203	CD	PRO	694	22.365	75.246	-1.206
204	C	PRO	694	22.661	72.720	1.398
205	O	PRO	694	22.222	73.405	2.316
206	CB	PRO	694	24.018	73.697	-0.465
207	CG	PRO	694	23.811	75.102	-0.777
208	N	ASP	695	23.175	71.516	1.550
209	CA	ASP	695	23.249	70.949	2.849
210	HN	ASP	695	23.510	71.006	0.757
211	C	ASP	695	24.549	71.260	3.463
212	O	ASP	695	25.441	71.872	2.877

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213	CB	ASP	695	23.090	69.450	2.784
214	CG	ASP	695	21.834	69.063	2.108
215	OD1	ASP	695	20.895	69.889	2.139
216	OD2	ASP	695	21.777	67.951	1.553
217	HD2	ASP	695	20.924	67.836	1.165
218	N	SER	696	24.636	70.819	4.690
219	CA	SER	696	25.822	70.972	5.447
220	HN	SER	696	23.847	70.365	5.104
221	C	SER	696	25.383	70.258	6.675
222	O	SER	696	24.203	70.267	7.041
223	CB	SER	696	26.139	72.446	5.692
224	OG	SER	696	25.437	73.057	6.764
225	HG	SER	696	25.733	73.975	6.792
226	N	PHE	697	26.530	69.629	7.299
227	CA	PHE	697	26.464	68.629	8.376
228	HN	PHE	697	27.449	69.713	6.888
229	C	PHE	697	25.787	69.190	9.644
230	O	PHE	697	24.983	68.458	10.181
231	CB	PHE	697	27.792	67.916	8.744
232	CG	PHE	697	28.885	68.879	9.171
233	CD1	PHE	697	29.085	69.233	10.558
234	CE1	PHE	697	30.116	70.166	10.939
235	CZ	PHE	697	30.974	70.747	9.940
236	CE2	PHE	697	30.793	70.386	8.561
237	CD2	PHE	697	30.762	69.457	8.182
238	N	ALA	698	26.114	70.494	10.112
239	CA	ALA	698	25.527	71.392	11.074
240	HN	ALA	698	27.103	70.500	9.969
241	C	ALA	698	24.166	71.500	10.449
242	O	ALA	698	23.510	70.508	10.391
243	CB	ALA	698	26.288	72.729	11.082
244	N	ALA	699	23.678	72.598	9.944
245	CA	ALA	699	22.339	72.472	9.371
246	HN	ALA	699	24.182	73.462	9.948
247	C	ALA	699	21.405	71.259	9.586
248	O	ALA	699	20.255	71.418	9.959
249	CB	ALA	699	22.524	72.827	7.885
250	N	LEU	700	21.874	70.055	9.313
251	CA	LEU	700	21.016	68.898	9.427
252	HN	LEU	700	22.825	69.943	9.027
253	C	LEU	700	20.937	68.217	10.741
254	O	LEU	700	19.955	67.556	11.097
255	CB	LEU	700	21.502	67.918	8.322
256	CG	LEU	700	21.248	68.304	6.839
257	CD1	LEU	700	21.362	67.062	5.944
258	CD2	LEU	700	19.881	68.973	6.626
259	N	LEU	701	22.241	67.945	11.274
260	CA	LEU	701	22.393	67.526	12.650
261	HN	LEU	701	23.099	68.182	10.776
262	C	LEU	701	21.407	68.489	13.358
263	O	LEU	701	20.678	68.015	14.213
264	CB	LEU	701	23.817	67.670	13.228
265	CG	LEU	701	24.838	66.645	12.675
266	CD1	LEU	701	26.284	67.148	12.829
267	CD2	LEU	701	24.711	65.277	13.353

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268	N	SER	702	21.348	69.874	12.942
269	CA	SER	702	20.571	70.736	13.707
270	HN	SER	702	21.934	70.156	12.182
271	C	SER	702	19.114	70.479	13.542
272	O	SER	702	18.437	70.227	14.534
273	CB	SER	702	20.916	72.229	13.479
274	OG	SER	702	21.723	72.780	14.526
275	HG	SER	702	21.208	72.741	15.337
276	N	SER	703	18.549	70.230	12.261
277	CA	SER	703	17.171	69.657	12.150
278	HN	SER	703	19.093	70.385	11.423
279	C	SER	703	16.944	68.360	13.073
280	O	SER	703	15.874	68.265	13.654
281	CB	SER	703	16.690	69.307	10.728
282	OG	SER	703	17.300	68.126	10.230
283	HG	SER	703	18.260	68.280	10.219
284	N	LEU	704	17.917	67.301	13.105
285	CA	LEU	704	17.740	65.962	13.703
286	HN	LEU	704	18.682	67.368	12.438
287	C	LEU	704	17.494	66.130	15.217
288	O	LEU	704	16.800	65.338	15.832
289	CB	LEU	704	18.981	65.050	13.574
290	CG	LEU	704	18.981	63.995	12.452
291	CD1	LEU	704	18.888	64.522	11.006
292	CD2	LEU	704	20.249	63.146	12.628
293	N	ASN	705	18.197	67.197	15.831
294	CA	ASN	705	18.013	67.600	17.218
295	HN	ASN	705	18.768	67.838	15.279
296	C	ASN	705	16.526	68.043	17.385
297	O	ASN	705	15.910	67.607	18.336
298	CB	ASN	705	18.960	68.709	17.715
299	CG	ASN	705	20.404	68.204	17.811
300	OD1	ASN	705	20.926	67.453	17.012
301	ND2	ASN	705	21.132	68.648	18.913
302	1HD2	ASN	705	21.930	68.109	19.248
303	2HD2	ASN	705	20.900	69.547	19.352
304	N	GLU	706	15.954	68.965	16.451
305	CA	GLU	706	14.614	69.578	16.579
306	HN	GLU	706	16.550	69.275	15.686
307	C	GLU	706	13.565	68.456	16.435
308	O	GLU	706	12.642	68.415	17.230
309	CB	GLU	706	14.253	70.731	15.602
310	CG	GLU	706	15.227	71.930	15.629
311	CD	GLU	706	15.722	72.275	17.032
312	OE1	GLU	706	15.056	72.441	18.043
313	OE2	GLU	706	17.073	72.369	17.008
314	HE2	GLU	706	17.366	72.541	17.911
315	N	LEU	707	13.710	67.522	15.388
316	CA	LEU	707	12.797	66.378	15.245
317	HN	LEU	707	14.627	67.512	14.939
318	C	LEU	707	12.929	65.492	16.540
319	O	LEU	707	11.940	65.187	17.173
320	CB	LEU	707	12.868	65.572	13.923
321	CG	LEU	707	11.772	64.471	13.807
322	CD1	LEU	707	10.351	64.964	14.105

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5	323	CD2	LEU	707	11.741	63.819	12.412
	324	N	GLY	708	14.203	65.213	17.065
	325	CA	GLY	708	14.409	64.586	18.375
	326	HN	GLY	708	15.077	65.405	16.550
	327	C	GLY	708	13.607	65.286	19.523
	328	O	GLY	708	13.223	64.551	20.422
	329	N	GLU	709	13.368	66.711	19.424
	330	CA	GLU	709	12.430	67.291	20.455
10	331	HN	GLU	709	13.232	66.870	18.416
	332	C	GLU	709	11.025	66.813	20.116
	333	O	GLU	709	10.470	66.147	20.971
	334	CB	GLU	709	12.087	68.724	20.989
	335	CG	GLU	709	11.457	69.883	20.147
	336	CD	GLU	709	10.300	70.500	20.944
15	337	OE1	GLU	709	9.121	70.204	20.833
	338	OE2	GLU	709	10.727	71.422	21.860
	339	HE2	GLU	709	10.002	71.760	22.412
	340	N	ARG	710	10.411	67.381	18.930
	341	CA	ARG	710	9.015	67.165	18.680
20	342	HN	ARG	710	11.030	67.728	18.226
	343	C	ARG	710	8.576	65.706	18.863
	344	O	ARG	710	7.454	65.462	19.302
	345	CB	ARG	710	8.675	67.723	17.311
	346	CG	ARG	710	9.112	69.185	17.218
	347	CD	ARG	710	8.843	69.723	15.849
25	348	NE	ARG	710	7.501	69.334	15.445
	349	CZ	ARG	710	7.222	68.779	14.275
	350	NH1	ARG	710	8.172	68.495	13.340
	351	1HH1	ARG	710	7.915	68.079	12.463
	352	2HH1	ARG	710	9.132	68.701	13.519
30	353	NH2	ARG	710	5.921	68.492	13.989
	354	1HH2	ARG	710	5.691	68.079	13.109
	355	2HH2	ARG	710	5.210	68.697	14.659
	356	HE	ARG	710	6.749	69.494	16.085
	357	N	GLN	711	9.493	64.717	18.415
35	358	CA	GLN	711	9.092	63.326	18.536
	359	HN	GLN	711	10.448	64.947	18.164
	360	C	GLN	711	8.965	62.993	20.054
	361	O	GLN	711	7.965	62.385	20.362
	362	CB	GLN	711	9.955	62.253	17.866
40	363	CG	GLN	711	9.197	60.900	17.986
	364	CD	GLN	711	9.873	59.707	17.350
	365	OE1	GLN	711	9.305	58.632	17.263
	366	NE2	GLN	711	11.203	59.917	16.945
	367	1HE2	GLN	711	11.810	59.096	17.046
	368	2HE2	GLN	711	11.540	60.821	17.305
45	369	N	LEU	712	10.009	63.314	20.993
	370	CA	LEU	712	10.114	62.841	22.369
	371	HN	LEU	712	10.567	64.088	20.697
	372	C	LEU	712	8.899	63.352	23.142
	373	O	LEU	712	8.473	62.756	24.139
50	374	CB	LEU	712	11.437	63.327	23.028
	375	CG	LEU	712	11.585	63.178	24.566
	376	CD1	LEU	712	12.902	63.812	25.033
	377	CD2	LEU	712	10.409	63.797	25.339

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378	N	VAL	713	8.336	64.448	22.642
379	CA	VAL	713	7.145	65.049	23.218
380	HN	VAL	713	8.748	64.876	21.837
381	C	VAL	713	5.974	64.150	22.835
382	O	VAL	713	5.085	63.912	23.641
383	CB	VAL	713	6.926	66.518	22.679
384	CG1	VAL	713	7.690	67.647	23.424
385	CG2	VAL	713	7.287	66.698	21.185
386	N	HIS	714	5.987	63.628	21.616
387	CA	HIS	714	4.923	62.724	21.198
388	HN	HIS	714	6.728	63.855	20.983
389	C	HIS	714	5.107	61.377	21.913
390	O	HIS	714	4.164	60.573	22.006
391	CB	HIS	714	4.961	62.530	19.673
392	CG	HIS	714	3.692	62.979	19.010
393	ND1	HIS	714	2.568	62.188	18.780
394	CE1	HIS	714	1.770	63.092	18.181
395	NE2	HIS	714	2.251	64.351	17.998
396	CD2	HIS	714	3.507	64.273	18.542
397	HE2	HIS	714	1.793	65.165	17.563
398	N	VAL	715	6.328	61.159	22.422
399	CA	VAL	715	6.725	59.930	23.143
400	HN	VAL	715	7.016	61.876	22.307
401	C	VAL	715	6.098	59.865	24.535
402	O	VAL	715	5.860	58.789	25.096
403	CB	VAL	715	8.302	59.868	23.233
404	CG1	VAL	715	8.899	58.734	24.112
405	CG2	VAL	715	9.004	59.733	21.861
406	N	VAL	716	5.853	61.042	25.092
407	CA	VAL	716	5.240	61.166	26.387
408	HN	VAL	716	6.102	61.873	24.594
409	C	VAL	716	3.724	60.950	26.214
410	O	VAL	716	3.127	60.223	27.013
411	CB	VAL	716	5.570	62.543	26.984
412	CG1	VAL	716	4.977	62.676	28.383
413	CG2	VAL	716	7.094	62.724	27.016
414	N	LYS	717	3.089	61.546	25.190
415	CA	LYS	717	1.644	61.294	25.014
416	HN	LYS	717	3.583	62.147	24.561
417	C	LYS	717	1.536	59.802	24.651
418	O	LYS	717	0.566	59.132	25.009
419	CB	LYS	717	0.962	62.138	23.883
420	CG	LYS	717	0.856	63.702	24.059
421	CD	LYS	717	-0.247	64.447	23.158
422	CE	LYS	717	-0.072	64.305	21.606
423	NZ	LYS	717	-0.903	65.223	20.724
424	HZ1	LYS	717	-0.504	66.172	20.745
425	HZ2	LYS	717	-0.896	64.869	19.757
426	HZ3	LYS	717	-1.844	65.248	21.062
427	N	TRP	718	2.523	59.265	23.943
428	CA	TRP	718	2.427	57.855	23.605
429	HN	TRP	718	3.307	59.813	23.652
430	C	TRP	718	2.530	57.001	24.873
431	O	TRP	718	1.646	56.190	25.144
432	CB	TRP	718	3.514	57.461	22.599

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433	CG	TRP	718	3.692	55.982	22.458
434	CD1	TRP	718	2.864	55.102	21.832
435	NE1	TRP	718	3.387	53.831	21.906
436	CE2	TRP	718	4.576	53.879	22.585
437	CD2	TRP	718	4.777	55.221	22.976
438	HE1	TRP	718	2.967	53.007	21.526
439	CE3	TRP	718	5.938	55.547	23.688
440	CZ3	TRP	718	6.813	54.537	24.037
441	CH2	TRP	718	6.583	53.207	23.640
442	CZ2	TRP	718	5.458	52.858	22.937
443	N	ALA	719	3.593	57.202	25.646
444	CA	ALA	719	3.823	56.439	26.880
445	HN	ALA	719	4.260	57.897	25.377
446	C	ALA	719	2.603	56.421	27.797
447	O	ALA	719	2.173	55.353	28.240
448	CB	ALA	719	5.039	57.001	27.626
449	N	LYS	720	2.056	57.602	28.074
450	CA	LYS	720	0.877	57.749	28.915
451	HN	LYS	720	2.473	58.425	27.688
452	C	LYS	720	-0.310	56.892	28.435
453	O	LYS	720	-1.087	56.394	29.246
454	CB	LYS	720	0.486	59.228	28.972
455	CG	LYS	720	1.490	60.104	29.739
456	CD	LYS	720	1.324	61.613	29.489
457	CE	LYS	720	-0.138	62.049	29.374
458	NZ	LYS	720	-0.392	63.445	29.911
459	HZ1	LYS	720	0.444	64.028	29.762
460	HZ2	LYS	720	-1.194	63.862	29.418
461	HZ3	LYS	720	-0.593	63.395	30.889
462	N	ALA	721	-0.447	56.695	27.130
463	CA	ALA	721	-1.556	55.887	26.617
464	HN	ALA	721	0.210	57.099	26.494
465	C	ALA	721	-1.321	54.381	26.706
466	O	ALA	721	-2.236	53.584	26.468
467	CB	ALA	721	-1.864	56.274	25.170
468	N	LEU	722	-0.098	53.982	27.036
469	CA	LEU	722	0.200	52.564	27.138
470	HN	LEU	722	0.617	54.658	27.214
471	C	LEU	722	-0.492	51.986	28.360
472	O	LEU	722	-0.279	52.425	29.492
473	CB	LEU	722	1.737	52.336	27.210
474	CG	LEU	722	2.576	52.603	25.931
475	CD1	LEU	722	4.062	52.733	26.293
476	CD2	LEU	722	2.397	51.510	24.865
477	N	PRO	723	-1.364	51.004	28.133
478	CA	PRO	723	-2.117	50.324	29.181
479	CD	PRO	723	-1.813	50.558	26.805
480	C	PRO	723	-1.207	49.971	30.340
481	O	PRO	723	-0.257	49.205	30.179
482	CB	PRO	723	-2.635	49.093	28.460
483	CG	PRO	723	-2.975	49.632	27.153
484	N	GLY	724	-1.488	50.541	31.504
485	CA	GLY	724	-0.686	50.263	32.676
486	HN	GLY	724	-2.263	51.169	31.573
487	C	GLY	724	0.523	51.152	32.913

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488	O	GLY	724	1.221	50.970	33.900
489	N	PHE	725	0.796	52.120	32.039
490	CA	PHE	725	1.967	52.963	32.256
491	HN	PHE	725	0.206	52.267	31.245
492	C	PHE	725	1.713	54.100	33.242
493	O	PHE	725	2.584	54.419	34.053
494	CB	PHE	725	2.474	53.554	30.937
495	CG	PHE	725	3.713	54.394	31.096
496	CD1	PHE	725	4.959	53.797	31.287
497	CE1	PHE	725	6.098	54.575	31.517
498	CZ	PHE	725	5.991	55.961	31.555
499	CE2	PHE	725	4.751	56.569	31.359
500	CD2	PHE	725	3.622	55.785	31.127
501	N	ARG	726	0.528	54.705	33.164
502	CA	ARG	726	0.150	55.833	34.029
503	HN	ARG	726	-0.133	54.378	32.488
504	C	ARG	726	0.050	55.468	35.498
505	O	ARG	726	0.346	56.277	36.381
506	CB	ARG	726	-1.197	56.436	33.600
507	CG	ARG	726	-1.155	57.242	32.317
508	CD	ARG	726	-2.138	58.410	32.336
509	NE	ARG	726	-1.902	59.315	33.460
510	CZ	ARG	726	-0.717	59.828	33.797
511	NH1	ARG	726	0.438	59.673	33.109
512	1HH1	ARG	726	1.279	60.106	33.442
513	2HH1	ARG	726	0.452	59.128	32.276
514	NH2	ARG	726	-0.677	60.598	34.918
515	1HH2	ARG	726	0.189	61.015	35.197
516	2HH2	ARG	726	-1.510	60.744	35.449
517	HE	ARG	726	-2.690	59.569	34.020
518	N	ASN	727	-0.380	54.242	35.752
519	CA	ASN	727	-0.544	53.777	37.110
520	HN	ASN	727	-0.595	53.628	34.993
521	C	ASN	727	0.765	53.516	37.822
522	O	ASN	727	0.778	53.044	38.950
523	CB	ASN	727	-1.436	52.541	37.106
524	CG	ASN	727	-2.805	52.837	36.517
525	OD1	ASN	727	-3.261	52.166	35.586
526	ND2	ASN	727	-3.556	53.863	37.133
527	1HD2	ASN	727	-4.491	54.048	36.802
528	2HD2	ASN	727	-3.175	54.391	37.903
529	N	LEU	728	1.882	53.801	37.176
530	CA	LEU	728	3.131	53.615	37.881
531	HN	LEU	728	1.864	54.134	36.233
532	C	LEU	728	3.372	54.966	38.511
533	O	LEU	728	2.730	55.960	38.163
534	CB	LEU	728	4.285	53.273	36.943
535	CG	LEU	728	4.343	51.909	36.258
536	CD1	LEU	728	4.962	52.123	34.901
537	CD2	LEU	728	5.151	50.896	37.058
538	N	HIS	729	4.308	55.000	39.441
539	CA	HIS	729	4.627	56.232	40.110
540	HN	HIS	729	4.799	54.162	39.683
541	C	HIS	729	5.054	57.283	39.094
542	O	HIS	729	5.887	57.008	38.239

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543	CB	HIS	729	5.742	55.981	41.108
544	CG	HIS	729	5.813	57.008	42.187
545	ND1	HIS	729	6.381	58.249	42.000
546	CE1	HIS	729	6.253	58.959	43.105
547	NE2	HIS	729	5.620	58.221	44.003
548	CD2	HIS	729	5.333	56.999	43.455
549	HE2	HIS	729	5.389	58.510	44.932
550	N	VAL	730	4.481	58.476	39.192
551	CA	VAL	730	4.812	59.579	38.294
552	HN	VAL	730	3.798	58.625	39.907
553	C	VAL	730	6.313	59.875	38.306
554	O	VAL	730	6.791	60.726	37.559
555	CB	VAL	730	3.984	60.854	38.725
556	CG1	VAL	730	3.709	61.905	37.614
557	CG2	VAL	730	2.598	60.527	39.330
558	N	ASP	731	7.044	59.181	39.173
559	CA	ASP	731	8.487	59.358	39.290
560	HN	ASP	731	6.589	58.516	39.764
561	C	ASP	731	9.214	58.319	38.448
562	O	ASP	731	10.326	58.562	37.974
563	CB	ASP	731	8.915	59.232	40.757
564	CG	ASP	731	9.276	60.572	41.382
565	OD1	ASP	731	8.645	61.590	41.021
566	OD2	ASP	731	10.184	60.599	42.245
567	HD2	ASP	731	10.306	61.486	42.548
568	N	ASP	732	8.597	57.155	38.283
569	CA	ASP	732	9.174	56.089	37.469
570	HN	ASP	732	7.714	57.004	38.728
571	C	ASP	732	8.833	56.439	36.039
572	O	ASP	732	9.643	56.265	35.127
573	CB	ASP	732	8.558	54.740	37.817
574	CG	ASP	732	8.720	54.394	39.271
575	OD1	ASP	732	9.723	54.839	39.871
576	OD2	ASP	732	7.853	53.670	39.809
577	HD2	ASP	732	8.076	53.532	40.717
578	N	GLN	733	7.603	56.922	35.872
579	CA	GLN	733	7.091	57.359	34.588
580	HN	GLN	733	7.005	56.988	36.671
581	C	GLN	733	8.131	58.302	34.013
582	O	GLN	733	8.317	58.385	32.802
583	CB	GLN	733	5.756	58.103	34.767
584	CG	GLN	733	4.525	57.204	34.669
585	CD	GLN	733	3.203	57.950	34.838
586	OE1	GLN	733	2.880	58.872	34.083
587	NE2	GLN	733	2.575	57.795	36.072
588	1HE2	GLN	733	1.680	58.234	36.220
589	2HE2	GLN	733	2.839	57.042	36.695
590	N	MET	734	8.829	59.003	34.899
591	CA	MET	734	9.852	59.943	34.473
592	HN	MET	734	8.647	58.882	35.875
593	C	MET	734	11.220	59.333	34.340
594	O	MET	734	12.079	59.902	33.666
595	CB	MET	734	9.951	61.118	35.433
596	CG	MET	734	9.164	62.319	34.998
597	SD	MET	734	9.654	63.746	35.952

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598	CE	MET	734	8.455	63.667	37.244
599	N	ALA	735	11.455	58.199	34.992
600	CA	ALA	735	12.771	57.598	34.869
601	HN	ALA	735	10.745	57.772	35.552
602	C	ALA	735	12.803	56.821	33.566
603	O	ALA	735	13.748	56.931	32.777
604	CB	ALA	735	13.083	56.721	36.094
605	N	VAL	736	11.744	56.053	33.341
606	CA	VAL	736	11.638	55.250	32.143
607	HN	VAL	736	11.004	56.030	34.013
608	C	VAL	736	11.833	56.098	30.863
609	O	VAL	736	12.645	55.741	30.008
610	CB	VAL	736	10.251	54.493	32.110
611	CG1	VAL	736	10.007	53.452	33.238
612	CG2	VAL	736	9.022	55.434	32.150
613	N	ILE	737	11.142	57.233	30.745
614	CA	ILE	737	11.297	58.090	29.570
615	HN	ILE	737	10.509	57.502	31.470
616	C	ILE	737	12.635	58.751	29.471
617	O	ILE	737	13.027	59.243	28.416
618	CB	ILE	737	10.118	59.146	29.580
619	CG1	ILE	737	8.725	58.571	29.167
620	CG2	ILE	737	10.413	60.390	28.685
621	CD1	ILE	737	7.530	59.536	29.307
622	N	GLN	738	13.337	58.801	30.584
623	CA	GLN	738	14.626	59.444	30.567
624	HN	GLN	738	12.981	58.399	31.427
625	C	GLN	738	15.719	58.459	30.267
626	O	GLN	738	16.740	58.801	29.672
627	CB	GLN	738	14.864	60.136	31.890
628	CG	GLN	738	14.349	61.550	31.885
629	CD	GLN	738	14.079	62.051	33.272
630	OE1	GLN	738	14.762	61.667	34.231
631	NE2	GLN	738	12.982	62.863	33.554
632	1HE2	GLN	738	12.838	63.166	34.506
633	2HE2	GLN	738	12.311	63.088	32.846
634	N	TYR	739	15.499	57.221	30.677
635	CA	TYR	739	16.473	56.184	30.422
636	HN	TYR	739	14.654	57.002	31.165
637	C	TYR	739	16.332	55.637	29.012
638	O	TYR	739	17.282	55.096	28.463
639	CB	TYR	739	16.270	55.032	31.377
640	CG	TYR	739	16.890	55.184	32.734
641	CD1	TYR	739	16.859	56.394	33.424
642	CE1	TYR	739	17.360	56.485	34.721
643	CZ	TYR	739	17.890	55.346	35.321
644	OH	TYR	739	18.388	55.465	36.601
645	HH	TYR	739	19.129	54.856	36.698
646	CE2	TYR	739	17.929	54.150	34.650
647	CD2	TYR	739	17.437	54.076	33.369
648	N	SER	740	15.157	55.784	28.406
649	CA	SER	740	14.983	55.203	27.088
650	HN	SER	740	14.411	56.282	28.849
651	C	SER	740	14.524	56.053	25.911
652	O	SER	740	14.159	55.506	24.878

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653	CB	SER	740	14.066	53.978	27.206
654	OG	SER	740	12.749	54.286	27.635
655	HG	SER	740	12.366	53.459	27.955
656	N	TRP	741	14.519	57.465	26.099
657	CA	TRP	741	14.133	58.264	24.924
658	HN	TRP	741	14.497	57.891	27.017
659	C	TRP	741	15.078	57.774	23.764
660	O	TRP	741	14.533	57.416	22.734
661	CB	TRP	741	14.133	59.797	25.069
662	CG	TRP	741	15.531	60.335	24.953
663	CD1	TRP	741	16.564	60.105	25.810
664	NE1	TRP	741	17.782	60.643	25.364
665	CE2	TRP	741	17.427	61.323	24.191
666	CD2	TRP	741	16.085	61.156	23.847
667	HE1	TRP	741	18.695	60.585	25.806
668	CE3	TRP	741	15.531	61.689	22.656
669	CZ3	TRP	741	16.425	62.386	21.792
670	CH2	TRP	741	17.785	62.601	22.177
671	CZ2	TRP	741	18.294	62.098	23.404
672	N	MET	742	16.511	57.700	23.949
673	CA	MET	742	17.460	57.375	22.864
674	HN	MET	742	16.918	58.325	24.642
675	C	MET	742	17.074	56.103	22.055
676	O	MET	742	17.258	56.121	20.863
677	CB	MET	742	18.909	57.247	23.380
678	CG	MET	742	19.989	56.973	22.306
679	SD	MET	742	20.191	58.185	20.942
680	CE	MET	742	19.820	59.767	21.764
681	N	GLY	743	16.525	54.998	22.724
682	CA	GLY	743	16.219	53.640	22.332
683	HN	GLY	743	16.635	55.206	23.696
684	C	GLY	743	14.879	53.727	21.599
685	O	GLY	743	14.703	53.142	20.535
686	N	LEU	744	13.800	54.496	22.119
687	CA	LEU	744	12.465	54.599	21.489
688	HN	LEU	744	13.971	55.061	22.943
689	C	LEU	744	12.576	55.382	20.155
690	O	LEU	744	12.106	54.862	19.151
691	CB	LEU	744	11.443	55.298	22.402
692	CG	LEU	744	11.169	54.461	23.672
693	CD1	LEU	744	10.761	55.334	24.862
694	CD2	LEU	744	10.137	53.369	23.354
695	N	MET	745	13.215	56.673	20.210
696	CA	MET	745	13.794	57.402	19.077
697	HN	MET	745	13.550	56.997	21.124
698	C	MET	745	14.432	56.310	18.190
699	O	MET	745	13.896	55.988	17.139
700	CB	MET	745	14.920	58.444	19.353
701	CG	MET	745	14.584	59.758	20.055
702	SD	MET	745	13.271	60.680	19.205
703	CE	MET	745	11.881	60.003	20.165
704	N	VAL	746	15.687	55.784	18.607
705	CA	VAL	746	16.555	55.323	17.526
706	HN	VAL	746	16.146	56.021	19.498
707	C	VAL	746	15.868	54.054	16.896

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708	O	VAL	746	15.708	54.010	15.695
709	CB	VAL	746	18.020	55.201	18.011
710	CG1	VAL	746	18.940	54.565	16.974
711	CG2	VAL	746	18.652	56.574	18.389
712	N	PHE	747	15.451	52.984	17.734
713	CA	PHE	747	14.928	51.646	17.382
714	HN	PHE	747	15.517	53.130	18.736
715	C	PHE	747	14.070	51.788	16.122
716	O	PHE	747	14.382	51.106	15.168
717	CB	PHE	747	14.101	51.009	18.516
718	CG	PHE	747	13.615	49.602	18.246
719	CD1	PHE	747	14.545	48.503	18.348
720	CE1	PHE	747	14.085	47.149	18.314
721	CZ	PHE	747	12.691	46.873	18.137
722	CE2	PHE	747	11.744	47.952	18.031
723	CD2	PHE	747	12.206	49.310	18.105
724	N	ALA	748	12.988	52.734	16.197
725	CA	ALA	748	11.929	53.166	15.258
726	HN	ALA	748	12.980	53.238	17.081
727	C	ALA	748	12.452	53.970	14.009
728	O	ALA	748	11.827	53.896	12.962
729	CB	ALA	748	10.866	54.042	15.955
730	N	MET	749	13.577	54.829	14.173
731	CA	MET	749	14.460	55.045	13.006
732	HN	MET	749	14.041	54.673	15.058
733	C	MET	749	14.556	53.699	12.250
734	O	MET	749	14.153	53.723	11.093
735	CB	MET	749	15.938	55.490	13.154
736	CG	MET	749	16.676	55.496	11.809
737	SD	MET	749	15.908	56.663	10.662
738	CE	MET	749	16.406	58.131	11.579
739	N	GLY	750	15.125	52.555	12.918
740	CA	GLY	750	15.233	51.315	12.206
741	HN	GLY	750	15.461	52.500	13.881
742	C	GLY	750	13.913	51.116	11.449
743	O	GLY	750	13.991	50.745	10.291
744	N	TRP	751	12.676	51.353	12.134
745	CA	TRP	751	11.460	50.940	11.462
746	HN	TRP	751	12.636	51.565	13.110
747	C	TRP	751	11.085	51.734	10.187
748	O	TRP	751	10.868	51.159	9.134
749	CB	TRP	751	10.334	50.995	12.476
750	CG	TRP	751	9.056	50.606	11.930
751	CD1	TRP	751	8.036	51.435	11.565
752	NE1	TRP	751	6.971	50.695	11.112
753	CE2	TRP	751	7.298	49.364	11.173
754	CD2	TRP	751	8.609	49.275	11.699
755	HE1	TRP	751	6.100	51.066	10.791
756	CE3	TRP	751	9.194	48.008	11.852
757	CZ3	TRP	751	8.448	46.879	11.513
758	CH2	TRP	751	7.139	47.004	11.001
759	CZ2	TRP	751	6.547	48.234	10.834
760	N	ARG	752	10.828	53.134	10.236
761	CA	ARG	752	10.481	53.916	9.023
762	HN	ARG	752	11.064	53.682	11.044

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763	C	ARG	752	11.467	53.500	7.878
764	O	ARG	752	11.091	53.384	6.727
765	CB	ARG	752	10.508	55.465	9.244
766	CG	ARG	752	9.234	55.992	9.981
767	CD	ARG	752	9.081	57.491	10.410
768	NE	ARG	752	10.218	58.276	10.932
769	CZ	ARG	752	11.005	57.728	11.925
770	NH1	ARG	752	10.676	56.604	12.600
771	1HH1	ARG	752	11.297	56.253	13.312
772	2HH1	ARG	752	9.810	56.136	12.400
773	NH2	ARG	752	12.193	58.225	12.333
774	1HH2	ARG	752	12.725	57.805	13.083
775	2HH2	ARG	752	12.508	59.058	11.877
776	HE	ARG	752	10.438	59.158	10.490
777	N	SER	753	12.832	53.352	8.234
778	CA	SER	753	13.858	53.113	7.230
779	HN	SER	753	13.094	53.305	9.198
780	C	SER	753	13.671	51.814	6.491
781	O	SER	753	13.787	51.732	5.269
782	CB	SER	753	15.220	53.082	7.901
783	OG	SER	753	15.598	54.311	8.521
784	HG	SER	753	16.377	54.104	9.055
785	N	PHE	754	13.406	50.789	7.273
786	CA	PHE	754	13.217	49.465	6.764
787	HN	PHE	754	13.334	50.941	8.259
788	C	PHE	754	11.985	49.344	5.896
789	O	PHE	754	11.951	48.557	4.958
790	CB	PHE	754	13.080	48.488	7.971
791	CG	PHE	754	12.144	47.285	7.775
792	CD1	PHE	754	12.430	46.341	6.782
793	CE1	PHE	754	11.651	45.196	6.657
794	CZ	PHE	754	10.592	44.977	7.535
795	CE2	PHE	754	10.309	45.908	8.534
796	CD2	PHE	754	11.081	47.060	8.653
797	N	THR	755	10.970	50.138	6.171
798	CA	THR	755	9.755	49.992	5.397
799	HN	THR	755	11.036	50.823	6.897
800	C	THR	755	9.638	50.815	4.144
801	O	THR	755	8.932	50.439	3.209
802	CB	THR	755	8.553	50.275	6.360
803	OG1	THR	755	8.606	49.415	7.490
804	HG1	THR	755	7.888	49.688	8.068
805	CG2	THR	755	7.141	50.057	5.774
806	N	ASN	756	10.347	51.932	4.147
807	CA	ASN	756	10.323	52.902	3.073
808	HN	ASN	756	10.933	52.116	4.936
809	C	ASN	756	11.405	52.732	2.021
810	O	ASN	756	11.350	53.354	0.962
811	CB	ASN	756	10.413	54.308	3.734
812	CG	ASN	756	9.814	55.482	2.952
813	OD1	ASN	756	10.054	56.646	3.238
814	ND2	ASN	756	9.001	55.229	1.962
815	1HD2	ASN	756	8.541	56.073	1.610
816	2HD2	ASN	756	8.750	54.253	1.807
817	N	VAL	757	12.404	51.906	2.311

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818	CA	VAL	757	13.501	51.711	1.378
819	HN	VAL	757	12.401	51.413	3.181
820	C	VAL	757	14.375	50.537	1.784
821	O	VAL	757	15.610	50.602	1.730
822	CB	VAL	757	14.355	53.036	1.271
823	CG1	VAL	757	14.528	53.853	2.581
824	CG2	VAL	757	15.790	52.817	0.734
825	N	ASN	758	13.702	49.482	2.233
826	CA	ASN	758	14.314	48.218	2.620
827	HN	ASN	758	12.708	49.561	2.310
828	C	ASN	758	15.612	48.239	3.458
829	O	ASN	758	16.410	47.298	3.378
830	CB	ASN	758	14.517	47.400	1.311
831	CG	ASN	758	13.894	47.971	0.033
832	OD1	ASN	758	14.553	48.581	-0.797
833	ND2	ASN	758	12.612	47.821	-0.165
834	1HD2	ASN	758	12.273	48.366	-0.962
835	2HD2	ASN	758	12.076	47.388	0.588
836	N	SER	759	15.798	49.283	4.266
837	CA	SER	759	16.988	49.450	5.119
838	HN	SER	759	15.092	49.990	4.295
839	C	SER	759	18.206	49.933	4.318
840	O	SER	759	19.349	49.548	4.604
841	CB	SER	759	17.291	48.133	5.878
842	OG	SER	759	17.771	47.094	5.019
843	HG	SER	759	17.071	46.891	4.393
844	N	ARG	760	17.949	50.786	3.330
845	CA	ARG	760	18.985	51.346	2.466
846	HN	ARG	760	16.999	51.058	3.171
847	C	ARG	760	19.341	52.784	2.844
848	O	ARG	760	20.516	53.158	2.902
849	CB	ARG	760	18.480	51.254	1.000
850	CG	ARG	760	18.391	49.814	0.428
851	CD	ARG	760	19.600	49.453	-0.445
852	NE	ARG	760	19.406	48.074	-0.963
853	CZ	ARG	760	20.247	47.425	-1.757
854	NH1	ARG	760	21.372	47.913	-2.190
855	1HH1	ARG	760	21.553	48.860	-1.855
856	2HH1	ARG	760	21.933	47.318	-2.796
857	NH2	ARG	760	19.923	46.235	-2.118
858	1HH2	ARG	760	19.025	45.948	-1.724
859	2HH2	ARG	760	20.563	45.732	-2.730
860	HE	ARG	760	18.572	47.596	-0.690
861	N	MET	761	18.293	53.567	3.089
862	CA	MET	761	18.370	54.983	3.462
863	HN	MET	761	17.384	53.158	3.015
864	C	MET	761	17.939	55.180	4.938
865	O	MET	761	17.228	54.341	5.487
866	CB	MET	761	17.443	55.779	2.503
867	CG	MET	761	18.096	56.281	1.198
868	SD	MET	761	19.267	55.055	0.591
869	CE	MET	761	20.100	56.069	-0.638
870	N	LEU	762	18.646	56.133	5.719
871	CA	LEU	762	18.008	56.502	6.977
872	HN	LEU	762	19.291	56.801	5.349

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873	C	LEU	762	16.874	57.403	6.518
874	O	LEU	762	17.022	58.280	5.682
875	CB	LEU	762	18.807	57.249	8.045
876	CG	LEU	762	19.912	56.413	8.714
877	CD1	LEU	762	20.320	57.178	9.974
878	CD2	LEU	762	19.487	54.969	9.048
879	N	TYR	763	15.670	57.231	7.238
880	CA	TYR	763	14.513	58.088	6.999
881	HN	TYR	763	15.561	56.388	7.766
882	C	TYR	763	13.906	58.809	8.186
883	O	TYR	763	12.846	58.426	8.682
884	CB	TYR	763	13.390	57.253	6.318
885	CG	TYR	763	13.796	56.416	5.099
886	CD1	TYR	763	13.972	57.016	3.849
887	CD2	TYR	763	14.003	55.040	5.240
888	CE1	TYR	763	14.356	56.247	2.753
889	CE2	TYR	763	14.386	54.274	4.144
890	CZ	TYR	763	14.563	54.878	2.901
891	OH	TYR	763	14.942	54.127	1.825
892	HH	TYR	763	15.040	53.217	2.109
893	N	PHE	764	14.785	59.734	8.835
894	CA	PHE	764	14.442	60.479	10.083
895	HN	PHE	764	15.772	59.742	8.578
896	C	PHE	764	12.936	60.840	10.052
897	O	PHE	764	12.200	60.760	11.025
898	CB	PHE	764	15.272	61.780	10.272
899	CG	PHE	764	16.672	61.362	10.642
900	CD1	PHE	764	17.646	60.998	9.635
901	CE1	PHE	764	18.897	60.394	10.028
902	CZ	PHE	764	19.179	60.161	11.424
903	CE2	PHE	764	18.228	60.565	12.429
904	CD2	PHE	764	16.976	61.155	12.037
905	N	ALA	765	12.573	61.312	8.769
906	CA	ALA	765	11.243	61.719	8.333
907	HN	ALA	765	13.221	61.061	8.011
908	C	ALA	765	11.117	61.299	6.822
909	O	ALA	765	12.084	61.094	6.089
910	CB	ALA	765	11.042	63.241	8.506
911	N	PRO	766	9.756	61.236	6.359
912	CA	PRO	766	9.578	61.215	4.895
913	CD	PRO	766	8.902	60.205	6.984
914	C	PRO	766	9.892	62.462	4.031
915	O	PRO	766	10.011	62.338	2.812
916	CB	PRO	766	8.151	60.692	4.748
917	CG	PRO	766	8.154	59.579	5.772
918	N	ASP	767	10.023	63.635	4.659
919	CA	ASP	767	10.402	64.883	3.987
920	HN	ASP	767	9.853	63.663	5.644
921	C	ASP	767	11.908	65.110	4.248
922	O	ASP	767	12.416	66.219	4.071
923	CB	ASP	767	9.546	66.079	4.513
924	CG	ASP	767	10.320	67.074	5.442
925	OD1	ASP	767	11.386	66.743	6.007
926	OD2	ASP	767	9.830	68.214	5.632
927	HD2	ASP	767	10.394	68.708	6.207

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928	N	LEU	768	12.622	64.067	4.686
929	CA	LEU	768	14.066	64.183	4.963
930	HN	LEU	768	12.166	63.188	4.829
931	C	LEU	768	14.766	62.853	5.221
932	O	LEU	768	14.844	62.374	6.362
933	CB	LEU	768	14.356	65.126	6.149
934	CG	LEU	768	15.833	65.518	6.400
935	CD1	LEU	768	15.922	66.481	7.567
936	CD2	LEU	768	16.695	64.304	6.705
937	N	VAL	769	15.303	62.307	4.134
938	CA	VAL	769	16.033	61.049	4.107
939	HN	VAL	769	15.198	62.798	3.270
940	C	VAL	769	17.515	61.321	3.918
941	O	VAL	769	17.910	62.236	3.195
942	CB	VAL	769	15.470	60.162	2.927
943	CG1	VAL	769	13.936	59.910	2.925
944	CG2	VAL	769	15.794	60.713	1.518
945	N	PHE	770	18.501	60.585	4.675
946	CA	PHE	770	19.970	60.640	4.547
947	HN	PHE	770	18.186	59.784	5.216
948	C	PHE	770	20.261	59.601	3.429
949	O	PHE	770	20.554	58.427	3.649
950	CB	PHE	770	20.836	60.221	5.758
951	CG	PHE	770	21.233	61.246	6.795
952	CD1	PHE	770	22.499	61.037	7.466
953	CE1	PHE	770	22.940	61.897	8.521
954	CZ	PHE	770	22.151	63.037	8.872
955	CE2	PHE	770	20.900	63.270	8.203
956	CD2	PHE	770	20.416	62.367	7.193
957	N	ASN	771	20.172	60.171	2.136
958	CA	ASN	771	20.583	59.440	0.952
959	HN	ASN	771	19.831	61.101	1.999
960	C	ASN	771	22.104	59.406	0.993
961	O	ASN	771	22.740	59.804	1.982
962	CB	ASN	771	20.157	60.228	-0.266
963	CG	ASN	771	20.462	61.686	-0.088
964	OD1	ASN	771	21.245	62.041	0.802
965	ND2	ASN	771	19.834	62.588	-0.969
966	1HD2	ASN	771	20.070	63.569	-0.935
967	2HD2	ASN	771	19.233	62.251	-1.704
968	N	GLU	772	22.663	58.979	-0.126
969	CA	GLU	772	24.082	58.822	-0.276
970	HN	GLU	772	22.072	58.756	-0.901
971	C	GLU	772	24.616	60.138	-0.412
972	O	GLU	772	25.341	60.550	0.437
973	CB	GLU	772	24.391	58.080	-1.511
974	CG	GLU	772	25.666	57.375	-1.442
975	CD	GLU	772	26.030	56.969	-2.820
976	OE1	GLU	772	25.501	55.939	-3.297
977	OE2	GLU	772	26.811	57.715	-3.446
978	HE2	GLU	772	26.969	57.356	-4.306
979	N	TYR	773	24.351	60.774	-1.523
980	CA	TYR	773	24.793	62.102	-1.541
981	HN	TYR	773	23.873	60.349	-2.292
982	C	TYR	773	25.042	62.437	-0.030

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983	O	TYR	773	26.119	62.188	0.452
984	CB	TYR	773	23.579	62.947	-2.027
985	CG	TYR	773	23.890	64.339	-2.587
986	CD1	TYR	773	22.957	65.375	-2.482
987	CD2	TYR	773	25.123	64.581	-3.202
988	CE1	TYR	773	23.258	66.640	-2.982
989	CE2	TYR	773	25.421	65.845	-3.701
990	CZ	TYR	773	24.488	66.874	-3.590
991	OH	TYR	773	24.780	68.116	-4.077
992	HH	TYR	773	25.661	68.094	-4.455
993	N	ARG	774	24.048	62.861	0.759
994	CA	ARG	774	24.284	63.236	2.187
995	HN	ARG	774	23.123	62.929	0.385
996	C	ARG	774	25.212	62.467	3.112
997	O	ARG	774	26.035	63.039	3.822
998	CB	ARG	774	22.962	63.385	2.896
999	CG	ARG	774	22.235	64.527	2.333
1000	CD	ARG	774	20.817	64.471	2.706
1001	NE	ARG	774	20.155	65.689	2.277
1002	CZ	ARG	774	18.843	65.836	2.288
1003	NH1	ARG	774	17.944	64.906	2.689
1004	1HH1	ARG	774	16.968	65.106	2.663
1005	2HH1	ARG	774	18.268	64.016	3.011
1006	NH2	ARG	774	18.393	67.046	1.851
1007	1HH2	ARG	774	17.416	67.245	1.824
1008	2HH2	ARG	774	19.071	67.726	1.561
1009	HE	ARG	774	20.718	66.451	1.959
1010	N	MET	775	24.911	61.105	3.376
1011	CA	MET	775	25.779	60.583	4.448
1012	HN	MET	775	24.830	60.517	2.549
1013	C	MET	775	27.305	60.651	4.013
1014	O	MET	775	28.147	60.293	4.826
1015	CB	MET	775	25.318	59.204	4.870
1016	CG	MET	775	25.815	58.802	6.270
1017	SD	MET	775	24.477	58.163	7.351
1018	CE	MET	775	25.415	57.094	8.481
1019	N	HIS	776	27.640	61.215	2.696
1020	CA	HIS	776	29.031	61.282	2.344
1021	HN	HIS	776	26.964	61.792	2.238
1022	C	HIS	776	29.746	62.384	3.101
1023	O	HIS	776	30.975	62.481	3.039
1024	CB	HIS	776	29.130	61.523	0.828
1025	CG	HIS	776	27.956	62.293	0.296
1026	ND1	HIS	776	26.766	61.743	-0.172
1027	CE1	HIS	776	26.107	62.869	-0.503
1028	NE2	HIS	776	26.735	64.060	-0.309
1029	CD2	HIS	776	27.943	63.678	0.215
1030	HE2	HIS	776	26.395	65.013	-0.501
1031	N	LYS	777	28.943	63.122	3.884
1032	CA	LYS	777	29.320	64.309	4.668
1033	HN	LYS	777	27.987	62.835	3.941
1034	C	LYS	777	30.189	64.269	5.882
1035	O	LYS	777	29.801	63.817	6.953
1036	CB	LYS	777	28.017	65.109	4.943
1037	CG	LYS	777	27.271	65.533	3.654

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1038	CD	LYS	777	27.913	66.694	2.890
1039	CE	LYS	777	27.075	67.006	1.644
1040	NZ	LYS	777	27.690	68.123	0.906
1041	HZ2	LYS	777	28.714	68.062	0.944
1042	HZ1	LYS	777	27.439	68.097	-0.088
1043	HZ3	LYS	777	27.389	68.991	1.303
1044	N	SER	778	31.289	64.992	5.774
1045	HN	SER	778	31.459	65.526	4.910
1046	CA	SER	778	32.264	65.049	6.850
1047	C	SER	778	32.066	64.179	8.078
1048	O	SER	778	32.971	63.485	8.496
1049	CB	SER	778	32.289	66.554	7.216
1050	OG	SER	778	32.013	67.404	6.097
1051	HG	SER	778	32.714	67.269	5.454
1052	N	ARG	779	31.042	64.493	9.064
1053	CA	ARG	779	31.023	63.897	10.434
1054	HN	ARG	779	30.246	65.047	8.755
1055	C	ARG	779	29.590	63.361	10.800
1056	O	ARG	779	28.841	63.946	11.571
1057	CB	ARG	779	31.557	64.839	11.534
1058	CG	ARG	779	33.073	65.106	11.405
1059	CD	ARG	779	33.744	65.498	12.728
1060	NE	ARG	779	33.977	64.443	13.758
1061	CZ	ARG	779	34.629	64.605	14.960
1062	NH1	ARG	779	35.116	65.817	15.379
1063	1HH1	ARG	779	34.981	66.593	14.763
1064	2HH1	ARG	779	35.591	65.928	16.255
1065	NH2	ARG	779	34.793	63.521	15.765
1066	1HH2	ARG	779	34.408	62.676	15.376
1067	2HH2	ARG	779	35.262	63.562	16.652
1068	HE	ARG	779	33.656	63.520	13.542
1069	N	MET	780	29.272	62.128	10.169
1070	CA	MET	780	27.864	61.726	9.970
1071	HN	MET	780	29.848	61.854	9.387
1072	C	MET	780	27.908	60.242	9.574
1073	O	MET	780	27.272	59.464	10.278
1074	CB	MET	780	27.041	62.330	8.814
1075	CG	MET	780	26.567	63.776	8.902
1076	SD	MET	780	25.378	64.019	7.543
1077	CE	MET	780	24.600	65.573	8.095
1078	N	TYR	781	28.649	59.894	8.359
1079	CA	TYR	781	28.868	58.454	8.021
1080	HN	TYR	781	29.099	60.596	7.760
1081	C	TYR	781	28.899	57.569	9.335
1082	O	TYR	781	28.171	56.608	9.513
1083	CB	TYR	781	30.119	58.165	7.148
1084	CG	TYR	781	30.298	56.667	7.018
1085	CD1	TYR	781	29.562	55.920	6.025
1086	CE1	TYR	781	29.644	54.479	6.002
1087	CZ	TYR	781	30.477	53.764	6.943
1088	OH	TYR	781	30.565	52.391	6.924
1089	HH	TYR	781	29.809	52.055	6.426
1090	CE2	TYR	781	31.236	54.523	7.898
1091	CD2	TYR	781	31.157	55.955	7.937
1092	N	SER	782	29.890	58.001	10.221

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1093	CA	SER	782	30.342	57.544	11.482
1094	HN	SER	782	30.414	58.669	9.692
1095	C	SER	782	29.351	57.385	12.601
1096	O	SER	782	29.510	56.535	13.475
1097	CB	SER	782	31.546	58.422	11.907
1098	OG	SER	782	32.608	57.663	12.495
1099	HG	SER	782	32.266	57.264	13.300
1100	N	GLN	783	28.232	58.202	12.588
1101	CA	GLN	783	27.423	58.261	13.809
1102	HN	GLN	783	28.195	58.944	11.888
1103	C	GLN	783	26.191	57.347	13.631
1104	O	GLN	783	25.946	56.384	14.349
1105	CB	GLN	783	27.169	59.738	14.096
1106	CG	GLN	783	28.525	60.430	14.416
1107	CD	GLN	783	29.225	59.669	15.557
1108	OE1	GLN	783	28.571	59.239	16.479
1109	NE2	GLN	783	30.618	59.475	15.570
1110	1HE2	GLN	783	30.948	59.552	16.532
1111	2HE2	GLN	783	31.148	59.941	14.847
1112	N	CYS	784	25.446	57.695	12.493
1113	CA	CYS	784	24.205	57.100	12.023
1114	HN	CYS	784	25.686	58.565	12.035
1115	C	CYS	784	24.455	55.669	11.442
1116	O	CYS	784	23.491	55.056	10.994
1117	CB	CYS	784	23.599	57.996	10.914
1118	SG	CYS	784	22.363	59.176	11.504
1119	HG	CYS	784	22.061	59.709	10.322
1120	N	VAL	785	25.779	55.124	11.438
1121	CA	VAL	785	25.912	53.807	11.104
1122	HN	VAL	785	26.470	55.639	11.944
1123	C	VAL	785	25.261	52.926	12.098
1124	O	VAL	785	24.784	51.860	11.743
1125	CB	VAL	785	27.461	53.505	11.015
1126	CG1	VAL	785	28.124	52.919	12.292
1127	CG2	VAL	785	27.846	52.534	9.872
1128	N	ARG	786	25.210	53.364	13.345
1129	CA	ARG	786	24.613	52.485	14.303
1130	HN	ARG	786	25.569	54.261	13.604
1131	C	ARG	786	23.134	52.462	14.182
1132	O	ARG	786	22.488	51.556	14.682
1133	CB	ARG	786	25.058	52.862	15.743
1134	CG	ARG	786	26.537	52.533	16.077
1135	CD	ARG	786	27.404	53.791	16.214
1136	NE	ARG	786	28.793	53.370	16.529
1137	CZ	ARG	786	29.821	54.186	16.714
1138	NH1	ARG	786	29.750	55.483	16.649
1139	1HH1	ARG	786	28.811	55.822	16.442
1140	2HH1	ARG	786	30.610	56.004	16.810
1141	NH2	ARG	786	30.962	53.653	16.975
1142	1HH2	ARG	786	30.910	52.633	17.003
1143	2HH2	ARG	786	31.757	54.274	17.115
1144	HE	ARG	786	28.967	52.388	16.607
1145	N	MET	787	22.362	53.565	13.664
1146	CA	MET	787	20.914	53.644	13.317
1147	HN	MET	787	22.895	54.316	13.257

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1148	C	MET	787	20.615	52.774	12.060
1149	O	MET	787	19.523	52.225	11.947
1150	CB	MET	787	20.545	55.080	12.895
1151	CG	MET	787	20.214	56.022	14.047
1152	SD	MET	787	19.941	57.729	13.485
1153	CE	MET	787	20.679	58.638	14.873
1154	N	ARG	788	21.643	52.808	11.071
1155	CA	ARG	788	21.545	52.016	9.879
1156	HN	ARG	788	22.321	53.542	11.110
1157	C	ARG	788	21.468	50.589	10.305
1158	O	ARG	788	20.835	49.738	9.690
1159	CB	ARG	788	22.833	52.293	9.056
1160	CG	ARG	788	22.708	53.433	8.011
1161	CD	ARG	788	24.063	53.832	7.411
1162	NE	ARG	788	23.839	54.942	6.450
1163	CZ	ARG	788	24.782	55.549	5.742
1164	NH1	ARG	788	26.046	55.246	5.791
1165	1HH1	ARG	788	26.249	54.481	6.435
1166	2HH1	ARG	788	26.675	55.784	5.199
1167	NH2	ARG	788	24.416	56.499	4.957
1168	1HH2	ARG	788	23.407	56.657	4.993
1169	2HH2	ARG	788	25.134	56.971	4.412
1170	HE	ARG	788	22.899	55.259	6.327
1171	N	HIS	789	22.153	50.339	11.396
1172	CA	HIS	789	22.243	49.017	11.904
1173	HN	HIS	789	22.616	51.086	11.873
1174	C	HIS	789	20.950	48.353	12.340
1175	O	HIS	789	20.775	47.145	12.174
1176	CB	HIS	789	23.254	49.033	13.063
1177	CG	HIS	789	23.245	47.752	13.845
1178	ND1	HIS	789	23.758	46.531	13.415
1179	CE1	HIS	789	23.365	45.744	14.434
1180	NE2	HIS	789	22.661	46.314	15.450
1181	CD2	HIS	789	22.586	47.627	15.060
1182	HE2	HIS	789	22.279	45.877	16.301
1183	N	LEU	790	20.049	49.131	12.906
1184	CA	LEU	790	18.817	48.561	13.415
1185	HN	LEU	790	20.216	50.114	12.985
1186	C	LEU	790	17.807	48.322	12.301
1187	O	LEU	790	17.107	47.307	12.280
1188	CB	LEU	790	18.223	49.485	14.515
1189	CG	LEU	790	19.132	50.595	15.108
1190	CD1	LEU	790	18.405	51.321	16.248
1191	CD2	LEU	790	20.478	50.052	15.615
1192	N	SER	791	17.761	49.278	11.384
1193	CA	SER	791	16.882	49.259	10.220
1194	HN	SER	791	18.369	50.064	11.497
1195	C	SER	791	17.248	48.056	9.390
1196	O	SER	791	16.448	47.474	8.650
1197	CB	SER	791	17.148	50.497	9.388
1198	OG	SER	791	17.297	50.290	8.012
1199	HG	SER	791	17.517	51.144	7.619
1200	N	GLN	792	18.510	47.706	9.525
1201	CA	GLN	792	19.063	46.614	8.791
1202	HN	GLN	792	19.094	48.216	10.156

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1203	C	GLN	792	18.670	45.295	9.410
1204	O	GLN	792	18.528	44.284	8.737
1205	CB	GLN	792	20.598	46.786	8.783
1206	CG	GLN	792	21.441	45.470	8.858
1207	CD	GLN	792	22.971	45.564	8.916
1208	OE1	GLN	792	23.661	44.562	9.015
1209	NE2	GLN	792	23.555	46.735	8.884
1210	2HE2	GLN	792	22.920	47.534	8.871
1211	1HE2	GLN	792	24.571	46.713	8.993
1212	N	GLU	793	18.482	45.308	10.714
1213	CA	GLU	793	18.132	44.091	11.393
1214	HN	GLU	793	18.582	46.159	11.228
1215	C	GLU	793	16.668	43.824	11.239
1216	O	GLU	793	16.230	42.679	11.129
1217	CB	GLU	793	18.518	44.229	12.845
1218	CG	GLU	793	19.997	44.150	12.996
1219	CD	GLU	793	20.469	42.740	12.723
1220	OE1	GLU	793	20.202	41.865	13.569
1221	OE2	GLU	793	21.081	42.493	11.663
1222	HE2	GLU	793	21.309	41.576	11.637
1223	N	PHE	794	15.909	44.900	11.228
1224	CA	PHE	794	14.477	44.796	11.066
1225	HN	PHE	794	16.330	45.802	11.332
1226	C	PHE	794	14.232	44.138	9.744
1227	O	PHE	794	13.408	43.246	9.581
1228	CB	PHE	794	13.862	46.228	11.037
1229	CG	PHE	794	13.638	46.904	12.399
1230	CD1	PHE	794	13.231	48.242	12.448
1231	CE1	PHE	794	13.102	48.891	13.671
1232	CZ	PHE	794	13.362	48.203	14.854
1233	CE2	PHE	794	13.757	46.867	14.813
1234	CD2	PHE	794	13.897	46.218	13.588
1235	N	GLY	795	14.976	44.617	8.782
1236	CA	GLY	795	14.838	44.102	7.476
1237	HN	GLY	795	15.639	45.342	8.971
1238	C	GLY	795	15.235	42.653	7.417
1239	O	GLY	795	14.511	41.796	6.912
1240	N	TRP	796	16.426	42.387	7.907
1241	CA	TRP	796	16.928	41.041	7.870
1242	HN	TRP	796	16.981	43.119	8.304
1243	C	TRP	796	16.024	40.070	8.594
1244	O	TRP	796	15.810	38.937	8.166
1245	CB	TRP	796	18.344	41.020	8.510
1246	CG	TRP	796	18.823	39.637	8.963
1247	CD1	TRP	796	20.079	39.349	9.535
1248	NE1	TRP	796	20.240	37.968	9.764
1249	CE2	TRP	796	20.240	37.968	9.764
1250	CD2	TRP	796	19.052	37.416	9.313
1251	HE1	TRP	796	18.184	38.423	8.823
1252	CE3	TRP	796	21.063	37.477	10.131
1253	CZ3	TRP	796	21.063	37.477	10.131
1254	CH2	TRP	796	16.916	38.084	8.283
1255	CZ2	TRP	796	16.542	36.740	8.264
1256	N	LEU	797	17.397	35.743	8.755
1257	CA	LEU	797	18.653	36.062	9.276
				15.495	40.520	9.712
				14.655	39.668	10.510

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1258	HN	LEU	797	15.677	41.458	10.007
1259	C	LEU	797	13.233	39.665	10.035
1260	O	LEU	797	12.396	38.918	10.547
1261	CB	LEU	797	14.713	40.140	11.936
1262	CG	LEU	797	15.052	39.039	12.925
1263	CD1	LEU	797	16.041	38.065	12.339
1264	CD2	LEU	797	15.612	39.703	14.158
1265	N	GLN	798	12.952	40.532	9.071
1266	CA	GLN	798	11.615	40.583	8.549
1267	HN	GLN	798	13.660	41.140	8.713
1268	C	GLN	798	10.695	40.731	9.721
1269	O	GLN	798	9.911	39.842	10.019
1270	CB	GLN	798	11.347	39.285	7.826
1271	CG	GLN	798	12.088	39.230	6.534
1272	CD	GLN	798	11.426	40.137	5.538
1273	OE1	GLN	798	12.016	41.104	5.053
1274	NE2	GLN	798	10.143	39.757	5.076
1275	1HE2	GLN	798	9.717	40.296	4.336
1276	2HE2	GLN	798	9.714	38.902	5.392
1277	N	ILE	799	10.802	41.849	10.410
1278	CA	ILE	799	9.957	42.060	11.554
1279	HN	ILE	799	11.465	42.546	10.139
1280	C	ILE	799	8.636	42.654	11.111
1281	O	ILE	799	8.601	43.514	10.245
1282	CB	ILE	799	10.695	42.984	12.606
1283	CG1	ILE	799	9.752	43.671	13.645
1284	CG2	ILE	799	11.563	44.092	11.934
1285	CD1	ILE	799	10.446	44.309	14.866
1286	N	THR	800	7.549	42.174	11.707
1287	CA	THR	800	6.206	42.646	11.374
1288	HN	THR	800	7.653	41.466	12.405
1289	C	THR	800	5.740	43.761	12.307
1290	O	THR	800	6.142	43.810	13.468
1291	CB	THR	800	5.226	41.426	11.437
1292	OG1	THR	800	4.904	41.115	12.786
1293	HG1	THR	800	4.250	40.410	12.749
1294	CG2	THR	800	5.748	40.098	10.847
1295	N	PRO	801	4.866	44.635	11.811
1296	CA	PRO	801	4.351	45.754	12.613
1297	C	PRO	801	3.904	45.330	13.998
1298	O	PRO	801	4.118	46.035	14.988
1299	CB	PRO	801	3.235	46.428	11.802
1300	CG	PRO	801	2.565	45.259	11.065
1301	CD	PRO	801	3.742	44.349	10.705
1302	N	GLN	802	3.249	44.186	14.073
1303	CA	GLN	802	2.791	43.772	15.369
1304	HN	GLN	802	3.079	43.631	13.259
1305	C	GLN	802	3.939	43.440	16.298
1306	O	GLN	802	3.917	43.859	17.456
1307	CB	GLN	802	1.795	42.595	15.279
1308	CG	GLN	802	0.278	42.976	15.236
1309	CD	GLN	802	-0.774	41.860	15.274
1310	OE1	GLN	802	-0.681	40.932	16.061
1311	NE2	GLN	802	-1.779	41.881	14.435
1312	2HE2	GLN	802	-1.761	42.646	13.759

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1313	1HE2	GLN	802	-2.397	41.069	14.483
1314	N	GLU	803	4.954	42.726	15.820
1315	CA	GLU	803	6.095	42.447	16.690
1316	HN	GLU	803	4.937	42.385	14.881
1317	C	GLU	803	6.767	43.775	17.046
1318	O	GLU	803	7.105	44.024	18.194
1319	CB	GLU	803	7.107	41.550	15.999
1320	CG	GLU	803	6.522	40.254	15.553
1321	CD	GLU	803	7.380	39.567	14.525
1322	OE1	GLU	803	7.888	40.268	13.614
1323	OE2	GLU	803	7.534	38.332	14.621
1324	HE2	GLU	803	8.090	38.028	13.920
1325	N	PHE	804	6.961	44.631	16.052
1326	CA	PHE	804	7.599	45.926	16.270
1327	HN	PHE	804	6.663	44.383	15.130
1328	C	PHE	804	6.929	46.789	17.341
1329	O	PHE	804	7.599	47.422	18.157
1330	CB	PHE	804	7.619	46.716	14.927
1331	CG	PHE	804	7.823	48.236	15.031
1332	CD1	PHE	804	9.111	48.750	15.221
1333	CE1	PHE	804	9.326	50.123	15.217
1334	CZ	PHE	804	8.259	50.993	15.006
1335	CE2	PHE	804	6.975	50.488	14.803
1336	CD2	PHE	804	6.757	49.113	14.818
1337	N	LEU	805	5.607	46.853	17.289
1338	CA	LEU	805	4.846	47.635	18.238
1339	HN	LEU	805	5.123	46.347	16.575
1340	C	LEU	805	5.157	47.193	19.666
1341	O	LEU	805	5.472	48.013	20.534
1342	CB	LEU	805	3.348	47.483	17.961
1343	CG	LEU	805	2.776	48.377	16.869
1344	CD1	LEU	805	1.284	48.208	16.796
1345	CD2	LEU	805	3.116	49.813	17.180
1346	N	CYS	806	5.049	45.885	19.882
1347	CA	CYS	806	5.314	45.273	21.168
1348	HN	CYS	806	4.771	45.298	19.122
1349	C	CYS	806	6.753	45.478	21.587
1350	O	CYS	806	7.049	45.668	22.759
1351	CB	CYS	806	5.047	43.781	21.103
1352	SG	CYS	806	3.280	43.364	20.905
1353	HG	CYS	806	3.138	42.037	20.857
1354	N	MET	807	7.657	45.430	20.633
1355	CA	MET	807	9.054	45.604	20.957
1356	HN	MET	807	7.378	45.273	19.686
1357	C	MET	807	9.406	47.017	21.406
1358	O	MET	807	10.286	47.205	22.252
1359	CB	MET	807	9.920	45.227	19.760
1360	CG	MET	807	10.038	43.744	19.538
1361	SD	MET	807	11.148	43.450	18.194
1362	CE	MET	807	10.046	43.456	16.968
1363	N	LYS	808	8.737	48.013	20.833
1364	CA	LYS	808	9.020	49.393	21.192
1365	HN	LYS	808	8.035	47.811	20.150
1366	C	LYS	808	8.475	49.690	22.582
1367	O	LYS	808	9.008	50.541	23.304

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1368	CB	LYS	808	8.393	50.324	20.170
1369	CG	LYS	808	8.973	51.714	20.152
1370	CD	LYS	808	8.430	52.481	18.948
1371	CE	LYS	808	6.976	52.947	19.146
1372	NZ	LYS	808	5.878	51.911	19.313
1373	HZ1	LYS	808	4.967	52.385	19.393
1374	HZ2	LYS	808	5.868	51.285	18.495
1375	HZ3	LYS	808	6.049	51.374	20.139
1376	N	ALA	809	7.405	48.990	22.947
1377	CA	ALA	809	6.794	49.152	24.249
1378	HN	ALA	809	7.011	48.333	22.304
1379	C	ALA	809	7.792	48.552	25.214
1380	O	ALA	809	8.098	49.138	26.238
1381	CB	ALA	809	5.433	48.434	24.276
1382	N	LEU	810	8.316	47.381	24.860
1383	CA	LEU	810	9.317	46.724	25.680
1384	HN	LEU	810	8.013	46.945	24.013
1385	C	LEU	810	10.541	47.619	25.856
1386	O	LEU	810	11.125	47.645	26.920
1387	CB	LEU	810	9.732	45.399	25.057
1388	CG	LEU	810	9.203	44.140	25.744
1389	CD1	LEU	810	8.142	44.484	26.747
1390	CD2	LEU	810	8.655	43.185	24.714
1391	N	LEU	811	10.939	48.369	24.839
1392	CA	LEU	811	12.106	49.226	25.037
1393	HN	LEU	811	10.456	48.350	23.963
1394	C	LEU	811	11.882	50.322	26.062
1395	O	LEU	811	12.836	50.825	26.638
1396	CB	LEU	811	12.541	49.892	23.740
1397	CG	LEU	811	13.182	49.049	22.650
1398	CD1	LEU	811	13.307	49.968	21.459
1399	CD2	LEU	811	14.549	48.490	23.053
1400	N	LEU	812	10.630	50.712	26.265
1401	CA	LEU	812	10.312	51.764	27.230
1402	HN	LEU	812	9.890	50.278	25.750
1403	C	LEU	812	10.574	51.184	28.611
1404	O	LEU	812	10.954	51.899	29.541
1405	CB	LEU	812	8.839	52.169	27.109
1406	CG	LEU	812	8.322	53.116	28.189
1407	CD1	LEU	812	9.120	54.420	28.142
1408	CD2	LEU	812	6.830	53.361	27.988
1409	N	PHE	813	10.381	49.872	28.710
1410	CA	PHE	813	10.577	49.134	29.944
1411	HN	PHE	813	10.089	49.370	27.896
1412	C	PHE	813	11.923	48.441	29.920
1413	O	PHE	813	12.131	47.479	30.657
1414	CB	PHE	813	9.458	48.055	30.068
1415	CG	PHE	813	8.019	48.533	29.822
1416	CD1	PHE	813	6.960	47.624	29.937
1417	CE1	PHE	813	5.660	48.020	29.640
1418	CZ	PHE	813	5.407	49.331	29.243
1419	CE2	PHE	813	6.455	50.245	29.139
1420	CD2	PHE	813	7.758	49.847	29.426
1421	N	SER	814	12.836	48.936	29.093
1422	CA	SER	814	14.140	48.299	28.921

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1423	HN	SER	814	12.627	49.766	28.575
1424	C	SER	814	15.279	48.552	29.904
1425	O	SER	814	16.359	47.972	29.754
1426	CB	SER	814	14.661	48.552	27.506
1427	OG	SER	814	15.276	49.824	27.308
1428	HG	SER	814	14.565	50.423	27.041
1429	N	ILE	815	15.084	49.428	30.877
1430	CA	ILE	815	16.134	49.624	31.870
1431	HN	ILE	815	14.231	49.947	30.930
1432	C	ILE	815	15.597	50.417	33.047
1433	O	ILE	815	14.769	51.313	32.899
1434	CB	ILE	815	17.441	50.281	31.265
1435	CG1	ILE	815	17.293	51.786	30.874
1436	CG2	ILE	815	17.986	49.509	30.023
1437	CD1	ILE	815	18.608	52.540	30.588
1438	N	ILE	816	16.033	50.023	34.233
1439	CA	ILE	816	15.585	50.666	35.447
1440	HN	ILE	816	16.684	49.266	34.291
1441	C	ILE	816	16.791	51.117	36.256
1442	O	ILE	816	17.930	50.741	35.961
1443	CB	ILE	816	14.666	49.671	36.266
1444	CG1	ILE	816	13.280	49.373	35.608
1445	CG2	ILE	816	14.415	50.145	37.730
1446	CD1	ILE	816	12.498	48.180	36.195
1447	N	PRO	817	16.563	51.958	37.275
1448	CA	PRO	817	17.668	52.431	38.099
1449	CD	PRO	817	15.276	52.418	37.819
1450	C	PRO	817	18.185	51.221	38.868
1451	O	PRO	817	17.402	50.334	39.217
1452	CB	PRO	817	16.993	53.465	38.993
1453	CG	PRO	817	15.648	52.866	39.206
1454	N	VAL	818	19.493	51.150	39.095
1455	CA	VAL	818	20.051	50.018	39.834
1456	HN	VAL	818	20.098	51.873	38.760
1457	C	VAL	818	19.707	50.210	41.288
1458	O	VAL	818	20.462	50.805	42.041
1459	CB	VAL	818	21.616	49.930	39.634
1460	CG1	VAL	818	22.412	49.182	40.739
1461	CG2	VAL	818	22.042	49.265	38.302
1462	N	ASP	819	18.554	49.692	41.671
1463	CA	ASP	819	18.050	49.804	43.023
1464	HN	ASP	819	18.004	49.200	40.995
1465	C	ASP	819	16.579	49.551	42.796
1466	O	ASP	819	15.893	48.957	43.627
1467	CB	ASP	819	18.259	51.217	43.592
1468	CG	ASP	819	19.591	51.361	44.337
1469	OD1	ASP	819	20.076	50.357	44.906
1470	OD2	ASP	819	20.141	52.485	44.364
1471	HD2	ASP	819	20.948	52.430	44.853
1472	N	GLY	820	16.109	50.000	41.634
1473	CA	GLY	820	14.719	49.790	41.279
1474	HN	GLY	820	16.717	50.483	41.004
1475	C	GLY	820	13.825	50.996	41.429
1476	O	GLY	820	14.203	52.016	42.013
1477	N	LEU	821	12.610	50.858	40.909

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1478	CA	LEU	821	11.630	51.928	40.943
1479	HN	LEU	821	12.363	49.989	40.480
1480	C	LEU	821	10.728	51.875	42.168
1481	O	LEU	821	10.668	50.869	42.873
1482	CB	LEU	821	10.747	51.874	39.691
1483	CG	LEU	821	11.282	51.133	38.465
1484	CD1	LEU	821	10.234	51.086	37.376
1485	CD2	LEU	821	12.499	51.831	37.961
1486	N	LYS	822	10.023	52.977	42.394
1487	CA	LYS	822	9.092	53.097	43.507
1488	HN	LYS	822	10.136	53.755	41.776
1489	C	LYS	822	7.993	52.055	43.370
1490	O	LYS	822	7.441	51.575	44.364
1491	CB	LYS	822	8.456	54.488	43.516
1492	CG	LYS	822	9.436	55.628	43.706
1493	CD	LYS	822	8.712	56.915	44.064
1494	CE	LYS	822	9.633	58.114	43.934
1495	NZ	LYS	822	9.044	59.459	44.297
1496	HZ1	LYS	822	9.774	60.183	44.231
1497	HZ2	LYS	822	8.277	59.685	43.648
1498	HZ3	LYS	822	8.690	59.427	45.232
1499	N	ASN	823	7.685	51.710	42.124
1500	CA	ASN	823	6.638	50.742	41.831
1501	HN	ASN	823	8.186	52.127	41.367
1502	C	ASN	823	7.218	49.524	41.124
1503	O	ASN	823	6.548	48.918	40.287
1504	CB	ASN	823	5.554	51.426	40.949
1505	CG	ASN	823	5.219	52.887	41.269
1506	OD1	ASN	823	5.671	53.817	40.618
1507	ND2	ASN	823	4.443	53.147	42.287
1508	1HD2	ASN	823	4.407	54.146	42.505
1509	2HD2	ASN	823	4.156	52.356	42.864
1510	N	GLN	824	8.456	49.178	41.466
1511	CA	GLN	824	9.149	48.037	40.861
1512	HN	GLN	824	8.931	49.716	42.162
1513	C	GLN	824	8.192	46.878	40.678
1514	O	GLN	824	8.146	46.244	39.621
1515	CB	GLN	824	10.317	47.597	41.749
1516	CG	GLN	824	11.125	46.435	41.192
1517	CD	GLN	824	11.753	46.736	39.838
1518	OE1	GLN	824	12.593	47.637	39.708
1519	NE2	GLN	824	11.300	46.051	38.710
1520	1HE2	GLN	824	11.713	46.227	37.809
1521	2HE2	GLN	824	10.698	45.239	38.819
1522	N	LYS	825	7.428	46.617	41.721
1523	CA	LYS	825	6.437	45.559	41.743
1524	HN	LYS	825	7.538	47.180	42.541
1525	C	LYS	825	5.617	45.521	40.432
1526	O	LYS	825	5.665	44.542	39.674
1527	CB	LYS	825	5.509	45.753	42.974
1528	CG	LYS	825	5.192	47.239	43.277
1529	CD	LYS	825	6.046	47.867	44.381
1530	CE	LYS	825	7.479	47.326	44.282
1531	NZ	LYS	825	8.344	48.054	45.227
1532	HZ2	LYS	825	7.837	48.262	46.095

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1533	HZ1	LYS	825	9.156	47.490	45.500
1534	HZ3	LYS	825	8.656	48.906	44.807
1535	N	PHE	826	4.911	46.618	40.171
1536	CA	PHE	826	4.043	46.821	39.000
1537	HN	PHE	826	4.976	47.370	40.826
1538	C	PHE	826	4.787	46.827	37.655
1539	O	PHE	826	4.284	46.363	36.626
1540	CB	PHE	826	3.299	48.180	39.169
1541	CG	PHE	826	1.789	48.172	38.885
1542	CD1	PHE	826	1.182	49.308	38.335
1543	CE1	PHE	826	-0.195	49.346	38.146
1544	CZ	PHE	826	-0.974	48.244	38.490
1545	CE2	PHE	826	-0.375	47.105	39.026
1546	CD2	PHE	826	1.002	47.069	39.226
1547	N	PHE	827	5.974	47.402	37.672
1548	CA	PHE	827	6.803	47.465	36.494
1549	HN	PHE	827	6.307	47.805	38.525
1550	C	PHE	827	6.951	46.051	35.974
1551	O	PHE	827	6.585	45.728	34.845
1552	CB	PHE	827	8.162	47.986	36.894
1553	CG	PHE	827	9.121	48.038	35.779
1554	CD1	PHE	827	9.173	49.152	34.962
1555	CE1	PHE	827	10.054	49.210	33.908
1556	CZ	PHE	827	10.896	48.134	33.652
1557	CE2	PHE	827	10.851	47.007	34.469
1558	CD2	PHE	827	9.958	46.962	35.523
1559	N	ASP	828	7.494	45.200	36.835
1560	CA	ASP	828	7.725	43.824	36.478
1561	HN	ASP	828	7.746	45.520	37.748
1562	C	ASP	828	6.457	43.114	36.085
1563	O	ASP	828	6.497	42.067	35.439
1564	CB	ASP	828	8.428	43.100	37.621
1565	CG	ASP	828	9.875	43.534	37.760
1566	OD1	ASP	828	10.488	43.887	36.727
1567	OD2	ASP	828	10.406	43.513	38.890
1568	HD2	ASP	828	11.302	43.807	38.823
1569	N	GLU	829	5.322	43.685	36.452
1570	CA	GLU	829	4.073	43.059	36.084
1571	HN	GLU	829	5.329	44.536	36.976
1572	C	GLU	829	3.716	43.494	34.675
1573	O	GLU	829	3.333	42.673	33.831
1574	CB	GLU	829	2.972	43.475	37.028
1575	CG	GLU	829	1.739	42.656	36.823
1576	CD	GLU	829	0.549	43.287	37.463
1577	OE1	GLU	829	0.751	44.056	38.432
1578	OE2	GLU	829	-0.580	43.009	37.001
1579	HE2	GLU	829	-1.243	43.470	37.491
1580	N	LEU	830	3.845	44.792	34.429
1581	CA	LEU	830	3.554	45.353	33.128
1582	HN	LEU	830	4.151	45.398	35.162
1583	C	LEU	830	4.558	44.788	32.155
1584	O	LEU	830	4.190	44.248	31.119
1585	CB	LEU	830	3.648	46.904	33.186
1586	CG	LEU	830	2.597	47.670	34.034
1587	CD1	LEU	830	2.769	49.183	33.847

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1588	CD2	LEU	830	1.153	47.266	33.696
1589	N	ARG	831	5.831	44.879	32.504
1590	CA	ARG	831	6.857	44.348	31.632
1591	HN	ARG	831	6.083	45.314	33.368
1592	C	ARG	831	6.663	42.886	31.230
1593	O	ARG	831	7.031	42.498	30.125
1594	CB	ARG	831	8.222	44.487	32.276
1595	CG	ARG	831	9.338	43.990	31.382
1596	CD	ARG	831	10.592	44.687	31.817
1597	NE	ARG	831	11.788	44.423	31.025
1598	CZ	ARG	831	12.240	43.212	30.720
1599	NH1	ARG	831	11.722	42.067	31.237
1600	1HH1	ARG	831	12.110	41.185	30.975
1601	2HH1	ARG	831	10.954	42.117	31.874
1602	NH2	ARG	831	13.301	43.102	29.867
1603	1HH2	ARG	831	13.666	42.201	29.627
1604	2HH2	ARG	831	13.711	43.925	29.480
1605	HE	ARG	831	12.305	45.210	30.688
1606	N	MET	832	6.107	42.067	32.117
1607	CA	MET	832	5.894	40.660	31.804
1608	HN	MET	832	5.830	42.421	33.011
1609	C	MET	832	4.759	40.503	30.792
1610	O	MET	832	4.808	39.640	29.913
1611	CB	MET	832	5.565	39.887	33.086
1612	CG	MET	832	5.557	38.364	32.952
1613	SD	MET	832	7.172	37.729	32.409
1614	CE	MET	832	6.700	37.034	30.872
1615	N	ASN	833	3.740	41.353	30.925
1616	CA	ASN	833	2.576	41.314	30.040
1617	HN	ASN	833	3.773	42.038	31.653
1618	C	ASN	833	2.939	41.645	28.607
1619	O	ASN	833	2.409	41.038	27.664
1620	CB	ASN	833	1.472	42.277	30.566
1621	CG	ASN	833	1.143	42.206	32.060
1622	OD1	ASN	833	1.580	43.017	32.863
1623	ND2	ASN	833	0.388	41.232	32.493
1624	1HD2	ASN	833	0.356	41.188	33.515
1625	2HD2	ASN	833	0.115	40.521	31.814
1626	N	TYR	834	3.812	42.633	28.428
1627	CA	TYR	834	4.212	42.934	27.078
1628	HN	TYR	834	4.177	43.149	29.204
1629	C	TYR	834	5.231	41.906	26.606
1630	O	TYR	834	5.482	41.819	25.421
1631	CB	TYR	834	4.742	44.368	26.937
1632	CG	TYR	834	3.624	45.390	27.002
1633	CD1	TYR	834	2.598	45.389	26.052
1634	CE1	TYR	834	1.490	46.230	26.193
1635	CZ	TYR	834	1.410	47.080	27.284
1636	OH	TYR	834	0.360	47.950	27.408
1637	HH	TYR	834	0.446	48.416	28.251
1638	CE2	TYR	834	2.427	47.107	28.224
1639	CD2	TYR	834	3.523	46.270	28.079
1640	N	ILE	835	5.828	41.106	27.485
1641	CA	ILE	835	6.748	40.123	26.919
1642	HN	ILE	835	5.659	41.174	28.468

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1643	C	ILE	835	5.924	39.010	26.292
1644	O	ILE	835	6.310	38.445	25.274
1645	CB	ILE	835	7.733	39.512	27.935
1646	CG2	ILE	835	8.465	38.324	27.285
1647	CG1	ILE	835	8.770	40.563	28.335
1648	CD1	ILE	835	9.397	40.319	29.678
1649	N	LYS	836	4.782	38.702	26.894
1650	CA	LYS	836	3.921	37.672	26.337
1651	HN	LYS	836	4.514	39.179	27.732
1652	C	LYS	836	3.173	38.282	25.150
1653	O	LYS	836	2.781	37.583	24.217
1654	CB	LYS	836	2.939	37.173	27.394
1655	CG	LYS	836	3.582	36.404	28.542
1656	CD	LYS	836	2.575	36.312	29.676
1657	CE	LYS	836	2.909	35.261	30.726
1658	NZ	LYS	836	1.798	35.031	31.736
1659	HZ1	LYS	836	1.400	35.937	32.021
1660	HZ2	LYS	836	1.061	34.451	31.310
1661	HZ3	LYS	836	2.168	34.562	32.538
1662	N	GLU	837	2.985	39.594	25.194
1663	CA	GLU	837	2.314	40.291	24.115
1664	HN	GLU	837	3.312	40.111	25.985
1665	C	GLU	837	3.224	40.145	22.892
1666	O	GLU	837	2.747	40.020	21.757
1667	CB	GLU	837	2.129	41.756	24.506
1668	CG	GLU	837	0.878	42.449	23.947
1669	CD	GLU	837	-0.363	41.556	23.874
1670	OE1	GLU	837	-0.768	40.962	24.903
1671	OE2	GLU	837	-0.936	41.463	22.763
1672	HE2	GLU	837	-1.683	40.889	22.841
1673	N	LEU	838	4.535	40.143	23.135
1674	CA	LEU	838	5.502	39.980	22.058
1675	HN	LEU	838	4.861	40.255	24.074
1676	C	LEU	838	5.325	38.560	21.578
1677	O	LEU	838	5.338	38.275	20.383
1678	CB	LEU	838	6.945	40.169	22.549
1679	CG	LEU	838	7.938	39.886	21.417
1680	CD1	LEU	838	7.511	40.699	20.219
1681	CD2	LEU	838	9.362	40.214	21.805
1682	N	ASP	839	5.140	37.669	22.539
1683	CA	ASP	839	4.962	36.262	22.235
1684	HN	ASP	839	5.124	37.971	23.492
1685	C	ASP	839	3.814	35.945	21.293
1686	O	ASP	839	3.991	35.178	20.350
1687	CB	ASP	839	4.836	35.497	23.579
1688	CG	ASP	839	4.904	33.965	23.509
1689	OD1	ASP	839	4.193	33.235	24.184
1690	OD2	ASP	839	5.821	33.516	22.599
1691	HD2	ASP	839	5.824	32.571	22.595
1692	N	ARG	840	2.640	36.517	21.558
1693	CA	ARG	840	1.457	36.297	20.722
1694	HN	ARG	840	2.563	37.116	22.355
1695	C	ARG	840	1.676	36.840	19.320
1696	O	ARG	840	1.331	36.197	18.326
1697	CB	ARG	840	0.244	36.979	21.411

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1698	CG	ARG	840	-0.080	36.454	22.835
1699	CD	ARG	840	-1.170	37.279	23.532
1700	NE	ARG	840	-1.819	36.423	24.557
1701	CZ	ARG	840	-2.807	36.797	25.359
1702	NH1	ARG	840	-3.350	37.978	25.353
1703	1HH1	ARG	840	-2.940	38.603	24.658
1704	2HH1	ARG	840	-4.102	38.147	26.018
1705	NH2	ARG	840	-3.253	35.929	26.197
1706	1HH2	ARG	840	-2.761	35.036	26.120
1707	2HH2	ARG	840	-4.009	36.210	26.817
1708	HE	ARG	840	-1.484	35.485	24.650
1709	N	ILE	841	2.213	38.053	19.254
1710	CA	ILE	841	2.476	38.694	17.985
1711	HN	ILE	841	2.440	38.534	20.101
1712	C	ILE	841	3.331	37.722	17.193
1713	O	ILE	841	3.092	37.505	16.007
1714	CB	ILE	841	3.218	40.072	18.222
1715	CG1	ILE	841	2.425	41.096	19.097
1716	CG2	ILE	841	3.618	40.780	16.891
1717	CD1	ILE	841	3.231	42.305	19.615
1718	N	ILE	842	4.316	37.130	17.862
1719	CA	ILE	842	5.197	36.165	17.212
1720	HN	ILE	842	4.456	37.350	18.827
1721	C	ILE	842	4.440	34.939	16.681
1722	O	ILE	842	4.598	34.576	15.516
1723	CB	ILE	842	6.304	35.673	18.167
1724	CG2	ILE	842	7.024	34.482	17.547
1725	CG1	ILE	842	7.295	36.803	18.451
1726	CD1	ILE	842	8.262	36.508	19.591
1727	N	ALA	843	3.624	34.300	17.528
1728	CA	ALA	843	2.864	33.114	17.116
1729	HN	ALA	843	3.529	34.639	18.464
1730	C	ALA	843	1.852	33.364	16.013
1731	O	ALA	843	1.584	32.470	15.219
1732	CB	ALA	843	2.243	32.446	18.355
1733	N	CYS	844	1.272	34.560	15.966
1734	CA	CYS	844	0.265	34.833	14.952
1735	HN	CYS	844	1.526	35.269	16.625
1736	C	CYS	844	0.809	35.417	13.651
1737	O	CYS	844	0.066	36.025	12.892
1738	CB	CYS	844	-0.847	35.704	15.569
1739	SG	CYS	844	-0.792	37.381	14.899
1740	HG	CYS	844	-0.268	37.965	15.973
1741	N	LYS	845	2.092	35.211	13.370
1742	CA	LYS	845	2.681	35.753	12.142
1743	HN	LYS	845	2.660	34.683	14.001
1744	C	LYS	845	3.342	34.641	11.356
1745	O	LYS	845	3.279	34.579	10.126
1746	CB	LYS	845	3.711	36.852	12.523
1747	CG	LYS	845	4.426	37.477	11.299
1748	CD	LYS	845	5.761	38.158	11.612
1749	CE	LYS	845	6.910	37.264	11.126
1750	NZ	LYS	845	7.238	37.604	9.730
1751	HZ2	LYS	845	7.153	38.616	9.574
1752	HZ1	LYS	845	8.209	37.362	9.506

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1753	HZ3	LYS	845	6.621	37.115	9.113
1754	N	ARG	846	3.975	33.764	12.123
1755	CA	ARG	846	4.743	32.640	11.628
1756	HN	ARG	846	3.917	33.887	13.114
1757	C	ARG	846	4.039	31.621	10.739
1758	O	ARG	846	3.938	31.802	9.526
1759	CB	ARG	846	5.417	31.956	12.850
1760	CG	ARG	846	6.967	31.902	12.795
1761	CD	ARG	846	7.587	33.235	12.356
1762	NE	ARG	846	7.062	34.308	13.238
1763	CZ	ARG	846	7.378	35.593	13.160
1764	NH1	ARG	846	8.199	36.095	12.285
1765	1HH1	ARG	846	8.584	35.395	11.650
1766	2HH1	ARG	846	8.364	37.099	12.325
1767	NH2	ARG	846	6.834	36.391	14.008
1768	1HH2	ARG	846	6.208	35.899	14.649
1769	2HH2	ARG	846	7.074	37.379	13.956
1770	HE	ARG	846	6.415	34.038	13.952
1771	N	LYS	847	3.544	30.551	11.345
1772	CA	LYS	847	2.923	29.508	10.561
1773	HN	LYS	847	3.601	30.466	12.339
1774	C	LYS	847	3.910	28.361	10.659
1775	O	LYS	847	4.792	28.190	9.811
1776	CB	LYS	847	2.682	29.909	9.080
1777	CG	LYS	847	2.106	28.759	8.216
1778	CD	LYS	847	1.917	29.098	6.735
1779	CE	LYS	847	1.412	27.855	5.992
1780	NZ	LYS	847	1.065	28.219	4.607
1781	HZ2	LYS	847	1.724	28.915	4.239
1782	HZ1	LYS	847	1.127	27.409	3.982
1783	HZ3	LYS	847	0.136	28.589	4.582
1784	N	ASN	848	3.755	27.613	11.746
1785	CA	ASN	848	4.563	26.452	12.119
1786	HN	ASN	848	3.014	27.868	12.368
1787	C	ASN	848	4.597	26.516	13.654
1788	O	ASN	848	3.550	26.710	14.274
1789	CB	ASN	848	5.977	26.531	11.523
1790	CG	ASN	848	6.207	25.526	10.393
1791	OD1	ASN	848	7.251	24.867	10.338
1792	ND2	ASN	848	5.198	25.367	9.416
1793	1HD2	ASN	848	5.373	24.776	8.619
1794	2HD2	ASN	848	4.431	26.024	9.406
1795	N	PRO	849	5.763	26.372	14.275
1796	CA	PRO	849	5.831	26.436	15.736
1797	C	PRO	849	7.207	26.150	16.311
1798	O	PRO	849	7.451	26.398	17.495
1799	CB	PRO	849	4.738	25.524	16.313
1800	CG	PRO	849	4.725	24.323	15.354
1801	CD	PRO	849	4.966	24.963	13.985
1802	N	THR	850	8.105	25.605	15.502
1803	CA	THR	850	9.441	25.356	16.017
1804	HN	THR	850	7.868	25.372	14.559
1805	C	THR	850	10.214	26.642	15.778
1806	O	THR	850	11.167	26.958	16.493
1807	CB	THR	850	10.126	24.154	15.283

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1808	OG1	THR	850	10.482	24.519	13.955
1809	HG1	THR	850	10.956	23.767	13.590
1810	CG2	THR	850	9.273	22.877	15.118
1811	N	SER	851	9.787	27.400	14.773
1812	CA	SER	851	10.446	28.655	14.481
1813	HN	SER	851	9.010	27.103	14.218
1814	C	SER	851	9.822	29.736	15.357
1815	O	SER	851	10.123	30.918	15.207
1816	CB	SER	851	10.338	29.008	12.977
1817	OG	SER	851	8.993	29.270	12.561
1818	HG	SER	851	8.491	28.460	12.686
1819	N	CYS	852	8.965	29.326	16.289
1820	CA	CYS	852	8.348	30.300	17.178
1821	HN	CYS	852	8.746	28.354	16.378
1822	C	CYS	852	9.238	30.709	18.333
1823	O	CYS	852	9.409	31.901	18.572
1824	CB	CYS	852	6.965	29.806	17.647
1825	SG	CYS	852	5.666	30.398	16.540
1826	HG	CYS	852	5.180	31.334	17.351
1827	N	SER	853	9.809	29.754	19.059
1828	CA	SER	853	10.721	30.160	20.111
1829	HN	SER	853	9.617	28.788	18.886
1830	C	SER	853	11.947	30.684	19.428
1831	O	SER	853	12.640	31.546	19.946
1832	CB	SER	853	11.052	28.960	21.034
1833	OG	SER	853	9.993	28.652	21.947
1834	HG	SER	853	9.878	29.413	22.522
1835	N	ARG	854	12.253	30.159	18.260
1836	CA	ARG	854	13.429	30.673	17.628
1837	HN	ARG	854	11.696	29.443	17.839
1838	C	ARG	854	13.229	32.139	17.268
1839	O	ARG	854	14.183	32.906	17.281
1840	CB	ARG	854	13.792	29.826	16.377
1841	CG	ARG	854	15.162	30.165	15.733
1842	CD	ARG	854	15.371	29.457	14.388
1843	NE	ARG	854	16.798	29.601	14.002
1844	CZ	ARG	854	17.349	29.113	12.899
1845	NH1	ARG	854	16.705	28.438	11.993
1846	1HH1	ARG	854	15.716	28.318	12.211
1847	2HH1	ARG	854	17.239	28.114	11.189
1848	NH2	ARG	854	18.605	29.324	12.720
1849	1HH2	ARG	854	19.015	29.862	13.486
1850	2HH2	ARG	854	19.036	28.950	11.876
1851	HE	ARG	854	17.393	30.108	14.626
1852	N	ARG	855	11.988	32.524	16.962
1853	CA	ARG	855	11.655	33.911	16.585
1854	HN	ARG	855	11.254	31.846	16.990
1855	C	ARG	855	11.888	34.813	17.795
1856	O	ARG	855	12.635	35.796	17.748
1857	CB	ARG	855	10.184	33.966	16.157
1858	CG	ARG	855	9.698	35.261	15.556
1859	CD	ARG	855	10.351	35.566	14.227
1860	NE	ARG	855	9.768	36.777	13.671
1861	CZ	ARG	855	10.332	37.527	12.738
1862	NH1	ARG	855	11.508	37.098	12.207

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1863	1HH1	ARG	855	11.953	37.643	11.499
1864	2HH1	ARG	855	11.913	36.244	12.526
1865	NH2	ARG	855	9.731	38.655	12.360
1866	1HH2	ARG	855	10.147	39.221	11.648
1867	2HH2	ARG	855	8.869	38.930	12.797
1868	HE	ARG	855	8.876	37.064	14.019
1869	N	PHE	856	11.215	34.449	18.875
1870	CA	PHE	856	11.305	35.136	20.138
1871	HN	PHE	856	10.612	33.655	18.811
1872	C	PHE	856	12.763	35.347	20.485
1873	O	PHE	856	13.213	36.471	20.731
1874	CB	PHE	856	10.664	34.278	21.208
1875	CG	PHE	856	10.553	34.946	22.519
1876	CD1	PHE	856	9.941	36.188	22.618
1877	CE1	PHE	856	9.787	36.809	23.842
1878	CZ	PHE	856	10.246	36.185	24.997
1879	CE2	PHE	856	10.863	34.944	24.911
1880	CD2	PHE	856	11.013	34.328	23.668
1881	N	TYR	857	13.497	34.247	20.513
1882	CA	TYR	857	14.903	34.289	20.828
1883	HN	TYR	857	13.067	33.367	20.311
1884	C	TYR	857	15.591	35.350	19.966
1885	O	TYR	857	16.340	36.174	20.483
1886	CB	TYR	857	15.511	32.908	20.612
1887	CG	TYR	857	16.991	32.859	20.832
1888	CD1	TYR	857	17.532	32.721	22.110
1889	CE1	TYR	857	18.909	32.720	22.307
1890	CZ	TYR	857	19.746	32.857	21.210
1891	OH	TYR	857	21.112	32.882	21.399
1892	HH	TYR	857	21.529	32.623	20.569
1893	CE2	TYR	857	19.221	32.991	19.936
1894	CD2	TYR	857	17.857	32.988	19.756
1895	N	GLN	858	15.322	35.361	18.668
1896	CA	GLN	858	15.949	36.355	17.800
1897	HN	GLN	858	14.689	34.689	18.283
1898	C	GLN	858	15.404	37.765	18.019
1899	O	GLN	858	16.168	38.739	18.044
1900	CB	GLN	858	15.752	36.015	16.334
1901	CG	GLN	858	16.085	34.612	15.954
1902	CD	GLN	858	15.869	34.395	14.479
1903	OE1	GLN	858	14.743	34.153	14.025
1904	NE2	GLN	858	17.014	34.493	13.651
1905	1HE2	GLN	858	16.916	34.308	12.664
1906	2HE2	GLN	858	17.927	34.643	14.051
1907	N	LEU	859	14.087	37.895	18.144
1908	CA	LEU	859	13.550	39.228	18.350
1909	HN	LEU	859	13.484	37.099	18.097
1910	C	LEU	859	14.160	39.797	19.635
1911	O	LEU	859	14.722	40.892	19.626
1912	CB	LEU	859	12.014	39.207	18.390
1913	CG	LEU	859	11.357	38.916	17.031
1914	CD1	LEU	859	9.853	39.037	17.129
1915	CD2	LEU	859	11.876	39.897	15.993
1916	N	THR	860	14.098	39.033	20.723
1917	CA	THR	860	14.656	39.500	21.990

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1918	HN	THR	860	13.667	38.132	20.673
1919	C	THR	860	16.176	39.693	21.962
1920	O	THR	860	16.754	40.268	22.890
1921	CB	THR	860	14.288	38.558	23.132
1922	OG1	THR	860	14.757	37.228	22.968
1923	HG1	THR	860	14.601	36.794	23.817
1924	CG2	THR	860	12.779	38.552	23.335
1925	N	LYS	861	16.830	39.216	20.907
1926	CA	LYS	861	18.270	39.397	20.817
1927	HN	LYS	861	16.336	38.737	20.182
1928	C	LYS	861	18.456	40.826	20.335
1929	O	LYS	861	19.325	41.553	20.810
1930	CB	LYS	861	18.892	38.425	19.817
1931	CG	LYS	861	20.364	38.109	20.110
1932	CD	LYS	861	20.502	37.119	21.279
1933	CE	LYS	861	21.959	36.933	21.747
1934	NZ	LYS	861	22.156	35.824	22.770
1935	HZ1	LYS	861	21.493	35.952	23.548
1936	HZ2	LYS	861	21.989	34.911	22.324
1937	HZ3	LYS	861	23.092	35.856	23.121
1938	N	LEU	862	17.603	41.223	19.396
1939	CA	LEU	862	17.635	42.565	18.843
1940	HN	LEU	862	16.918	40.577	19.059
1941	C	LEU	862	17.397	43.581	19.962
1942	O	LEU	862	18.051	44.628	20.021
1943	CB	LEU	862	16.553	42.714	17.782
1944	CG	LEU	862	16.934	43.629	16.630
1945	CD1	LEU	862	15.660	44.226	16.085
1946	CD2	LEU	862	17.893	44.732	17.085
1947	N	LEU	863	16.452	43.267	20.842
1948	CA	LEU	863	16.140	44.140	21.963
1949	HN	LEU	863	15.944	42.412	20.731
1950	C	LEU	863	17.379	44.403	22.790
1951	O	LEU	863	17.776	45.549	22.950
1952	CB	LEU	863	15.043	43.515	22.829
1953	CG	LEU	863	13.714	43.547	22.073
1954	CD1	LEU	863	12.587	43.029	22.926
1955	CD2	LEU	863	13.447	44.988	21.639
1956	N	ASP	864	17.999	43.343	23.298
1957	CA	ASP	864	19.198	43.467	24.125
1958	HN	ASP	864	17.634	42.432	23.108
1959	C	ASP	864	20.327	44.239	23.470
1960	O	ASP	864	21.122	44.895	24.145
1961	CB	ASP	864	19.733	42.092	24.495
1962	CG	ASP	864	18.831	41.367	25.445
1963	OD1	ASP	864	17.986	42.034	26.080
1964	OD2	ASP	864	18.971	40.138	25.571
1965	HD2	ASP	864	18.343	39.811	26.197
1966	N	SER	865	20.400	44.148	22.152
1967	CA	SER	865	21.458	44.813	21.411
1968	HN	SER	865	19.714	43.614	21.657
1969	C	SER	865	21.136	46.275	21.164
1970	O	SER	865	21.914	47.011	20.551
1971	CB	SER	865	21.676	44.093	20.087
1972	OG	SER	865	21.198	44.768	18.923

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1973	HG	SER	865	20.247	44.893	19.052
1974	N	VAL	866	19.975	46.683	21.653
1975	CA	VAL	866	19.504	48.049	21.499
1976	HN	VAL	866	19.402	46.028	22.145
1977	C	VAL	866	20.218	48.908	22.537
1978	O	VAL	866	20.382	50.115	22.363
1979	CB	VAL	866	17.942	48.064	21.735
1980	CG1	VAL	866	17.131	49.109	20.919
1981	CG2	VAL	866	17.252	46.706	21.460
1982	N	GLN	867	20.636	48.265	23.626
1983	CA	GLN	867	21.366	48.965	24.663
1984	HN	GLN	867	20.445	47.289	23.728
1985	C	GLN	867	22.676	49.372	24.018
1986	O	GLN	867	23.069	50.525	24.094
1987	CB	GLN	867	21.611	48.048	25.882
1988	CG	GLN	867	20.397	47.844	26.848
1989	CD	GLN	867	19.936	46.419	27.177
1990	OE1	GLN	867	18.987	46.219	27.919
1991	NE2	GLN	867	20.578	45.392	26.680
1992	2HE2	GLN	867	21.402	45.627	26.124
1993	1HE2	GLN	867	20.246	44.480	27.000
1994	N	PRO	868	23.343	48.454	23.333
1995	CA	PRO	868	24.594	48.867	22.735
1996	C	PRO	868	24.485	49.904	21.618
1997	O	PRO	868	25.405	50.714	21.471
1998	CB	PRO	868	25.417	47.634	22.332
1999	CG	PRO	868	24.369	46.674	21.747
2000	CD	PRO	868	23.150	46.894	22.646
2001	N	ILE	869	23.417	49.918	20.817
2002	CA	ILE	869	23.396	50.978	19.804
2003	HN	ILE	869	22.679	49.248	20.903
2004	C	ILE	869	23.025	52.308	20.464
2005	O	ILE	869	23.534	53.352	20.062
2006	CB	ILE	869	22.493	50.676	18.539
2007	CG1	ILE	869	21.636	49.374	18.647
2008	CG2	ILE	869	23.313	50.609	17.214
2009	CD1	ILE	869	20.519	49.215	17.595
2010	N	ALA	870	22.176	52.274	21.495
2011	CA	ALA	870	21.805	53.511	22.196
2012	HN	ALA	870	21.790	51.400	21.791
2013	C	ALA	870	23.037	54.118	22.876
2014	O	ALA	870	23.216	55.331	22.884
2015	CB	ALA	870	20.651	53.247	23.179
2016	N	ARG	871	23.895	53.278	23.440
2017	CA	ARG	871	25.100	53.794	24.070
2018	HN	ARG	871	23.715	52.294	23.431
2019	C	ARG	871	25.856	54.646	23.041
2020	O	ARG	871	26.083	55.831	23.258
2021	CB	ARG	871	25.980	52.625	24.594
2022	CG	ARG	871	27.191	53.058	25.463
2023	CD	ARG	871	27.897	51.866	26.122
2024	NE	ARG	871	26.863	50.904	26.580
2025	CZ	ARG	871	27.100	49.752	27.193
2026	NH1	ARG	871	28.286	49.306	27.482
2027	1HH1	ARG	871	29.033	49.937	27.192

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2028	2HH1	ARG	871	28.340	48.405	27.955
2029	NH2	ARG	871	26.084	49.034	27.519
2030	1HH2	ARG	871	25.203	49.473	27.247
2031	2HH2	ARG	871	26.259	48.147	27.987
2032	HE	ARG	871	25.907	51.146	26.412
2033	N	GLU	872	26.408	53.950	21.931
2034	CA	GLU	872	27.385	54.484	20.981
2035	HN	GLU	872	26.260	52.944	21.910
2036	C	GLU	872	26.849	55.815	20.337
2037	O	GLU	872	27.667	56.632	19.950
2038	CB	GLU	872	27.726	53.433	19.901
2039	CG	GLU	872	28.328	52.104	20.449
2040	CD	GLU	872	28.409	51.032	19.362
2041	OE1	GLU	872	29.430	50.652	18.829
2042	OE2	GLU	872	27.203	50.544	18.978
2043	HE2	GLU	872	27.293	50.078	18.137
2044	N	LEU	873	25.436	56.022	20.276
2045	CA	LEU	873	24.724	57.200	19.760
2046	HN	LEU	873	24.861	55.285	20.690
2047	C	LEU	873	24.595	58.270	20.894
2048	O	LEU	873	25.019	59.379	20.636
2049	CB	LEU	873	23.337	56.855	19.192
2050	CG	LEU	873	23.378	55.882	17.985
2051	CD1	LEU	873	22.002	55.231	17.841
2052	CD2	LEU	873	23.780	56.573	16.663
2053	N	HIS	874	23.965	57.966	22.145
2054	CA	HIS	874	24.158	58.786	23.367
2055	HN	HIS	874	23.560	57.051	22.324
2056	C	HIS	874	25.542	59.472	23.379
2057	O	HIS	874	25.571	60.658	23.626
2058	CB	HIS	874	24.234	58.102	24.741
2059	CG	HIS	874	22.936	57.702	25.317
2060	ND1	HIS	874	22.813	56.503	25.961
2061	CE1	HIS	874	21.722	56.586	26.613
2062	NE2	HIS	874	20.972	57.795	26.378
2063	CD2	HIS	874	21.766	58.465	25.455
2064	HE2	HIS	874	20.081	58.130	26.741
2065	N	GLN	875	26.721	58.681	23.357
2066	CA	GLN	875	28.044	59.302	23.396
2067	HN	GLN	875	26.630	57.688	23.284
2068	C	GLN	875	28.165	60.488	22.389
2069	O	GLN	875	28.635	61.533	22.815
2070	CB	GLN	875	29.172	58.270	23.174
2071	CG	GLN	875	29.403	57.239	24.328
2072	CD	GLN	875	28.824	57.531	25.718
2073	OE1	GLN	875	28.948	56.733	26.633
2074	NE2	GLN	875	28.161	58.640	25.931
2075	2HE2	GLN	875	28.033	59.231	25.108
2076	1HE2	GLN	875	27.754	58.726	26.864
2077	N	PHE	876	27.718	60.280	21.057
2078	CA	PHE	876	27.841	61.462	20.165
2079	HN	PHE	876	26.885	59.685	20.995
2080	C	PHE	876	26.792	62.593	20.503
2081	O	PHE	876	27.169	63.758	20.556
2082	CB	PHE	876	27.834	61.063	18.696

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2083	CG	PHE	876	28.247	62.231	17.831
2084	CD1	PHE	876	27.246	63.136	17.335
2085	CE1	PHE	876	27.575	64.131	16.353
2086	CZ	PHE	876	28.931	64.264	15.911
2087	CE2	PHE	876	29.959	63.443	16.484
2088	CD2	PHE	876	29.624	62.433	17.447
2089	N	THR	877	25.428	62.231	20.747
2090	CA	THR	877	24.359	63.113	21.226
2091	HN	THR	877	25.102	61.272	20.752
2092	C	THR	877	24.977	64.063	22.321
2093	O	THR	877	24.824	65.272	22.274
2094	CB	THR	877	23.155	62.343	21.893
2095	OG1	THR	877	22.571	61.260	21.154
2096	HG1	THR	877	21.647	61.493	20.956
2097	CG2	THR	877	22.055	63.305	22.371
2098	N	PHE	878	25.576	63.410	23.433
2099	CA	PHE	878	25.950	64.048	24.711
2100	HN	PHE	878	25.863	62.435	23.355
2101	C	PHE	878	27.225	64.946	24.507
2102	O	PHE	878	27.176	66.082	24.911
2103	CB	PHE	878	26.189	63.055	25.877
2104	CG	PHE	878	24.941	62.370	26.424
2105	CD1	PHE	878	23.710	62.202	25.690
2106	CE1	PHE	878	22.579	61.526	26.255
2107	CZ	PHE	878	22.652	60.972	27.569
2108	CE2	PHE	878	23.846	61.156	28.333
2109	CD2	PHE	878	24.980	61.840	27.762
2110	N	ASP	879	28.404	64.415	23.941
2111	CA	ASP	879	29.580	65.087	23.411
2112	HN	ASP	879	28.357	63.418	23.880
2113	C	ASP	879	29.097	66.302	22.642
2114	O	ASP	879	29.026	67.386	23.195
2115	CB	ASP	879	30.337	64.088	22.498
2116	CG	ASP	879	31.786	64.445	22.138
2117	OD1	ASP	879	32.533	63.682	21.542
2118	OD2	ASP	879	32.135	65.707	22.532
2119	HD2	ASP	879	33.032	65.877	22.288
2120	N	LEU	880	28.746	66.177	21.254
2121	CA	LEU	880	28.095	67.195	20.392
2122	HN	LEU	880	28.531	65.227	20.984
2123	C	LEU	880	27.516	68.324	21.297
2124	O	LEU	880	27.833	69.492	21.123
2125	CB	LEU	880	26.987	66.542	19.521
2126	CG	LEU	880	26.285	67.339	18.404
2127	CD1	LEU	880	27.309	67.731	17.314
2128	CD2	LEU	880	25.111	66.489	17.844
2129	N	LEU	881	26.617	67.870	22.315
2130	CA	LEU	881	25.882	68.810	23.169
2131	HN	LEU	881	26.432	66.890	22.389
2132	C	LEU	881	26.754	69.636	24.119
2133	O	LEU	881	26.385	70.749	24.493
2134	CB	LEU	881	24.799	68.018	23.956
2135	CG	LEU	881	23.904	68.799	24.955
2136	CD1	LEU	881	22.656	69.333	24.239
2137	CD2	LEU	881	23.483	67.949	26.165

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2138	N	ILE	882	27.893	69.086	24.527
2139	CA	ILE	882	28.793	69.797	25.426
2140	HN	ILE	882	28.136	68.169	24.212
2141	C	ILE	882	29.999	70.348	24.666
2142	O	ILE	882	31.141	70.250	25.129
2143	CB	ILE	882	29.229	68.835	26.606
2144	CG1	ILE	882	28.050	68.094	27.312
2145	CG2	ILE	882	30.069	69.563	27.700
2146	CD1	ILE	882	28.437	67.190	28.501
2147	N	LYS	883	29.736	70.910	23.488
2148	CA	LYS	883	30.771	71.515	22.651
2149	HN	LYS	883	28.791	70.918	23.162
2150	C	LYS	883	30.117	72.518	21.717
2151	O	LYS	883	29.586	72.137	20.671
2152	CB	LYS	883	31.531	70.422	21.850
2153	CG	LYS	883	32.746	70.970	21.061
2154	CD	LYS	883	33.247	70.060	19.935
2155	CE	LYS	883	34.398	70.755	19.197
2156	NZ	LYS	883	34.996	69.818	18.229
2157	HZ2	LYS	883	34.272	69.230	17.800
2158	HZ1	LYS	883	35.451	70.319	17.459
2159	HZ3	LYS	883	35.667	69.241	18.695
2160	N	SER	884	28.420	72.393	21.414
2161	CA	SER	884	27.396	72.888	20.489
2162	HN	SER	884	28.135	72.067	22.315
2163	C	SER	884	27.610	74.331	20.042
2164	O	SER	884	27.438	74.658	18.872
2165	CB	SER	884	26.017	72.756	21.129
2166	OG	SER	884	25.870	73.467	22.358
2167	HG	SER	884	24.943	73.377	22.616
2168	N	HIS	885	27.987	75.188	20.985
2169	CA	HIS	885	28.234	76.608	20.719
2170	HN	HIS	885	28.107	74.850	21.918
2171	C	HIS	885	29.414	76.858	19.764
2172	O	HIS	885	29.555	77.954	19.228
2173	CB	HIS	885	28.426	77.340	22.060
2174	CG	HIS	885	29.180	78.638	21.969
2175	ND1	HIS	885	28.563	79.849	21.732
2176	CE1	HIS	885	29.462	80.820	21.769
2177	NE2	HIS	885	30.643	80.282	22.016
2178	CD2	HIS	885	30.496	78.918	22.141
2179	HE2	HIS	885	31.505	80.783	22.098
2180	N	MET	886	31.650	74.889	20.070
2181	CA	MET	886	32.565	75.329	19.028
2182	HN	MET	886	31.962	74.238	20.761
2183	C	MET	886	31.840	74.738	17.822
2184	O	MET	886	31.805	75.321	16.735
2185	CB	MET	886	33.963	74.675	19.210
2186	CG	MET	886	34.261	74.102	20.611
2187	SD	MET	886	36.001	73.655	20.730
2188	CE	MET	886	35.927	72.697	22.250
2189	N	VAL	887	31.241	73.571	18.051
2190	CA	VAL	887	30.508	72.855	17.019
2191	HN	VAL	887	31.297	73.172	18.966
2192	C	VAL	887	29.274	73.631	16.592

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2193	O	VAL	887	28.923	73.650	15.414
2194	CB	VAL	887	30.115	71.415	17.537
2195	CG1	VAL	887	30.240	70.255	16.511
2196	CG2	VAL	887	30.919	70.953	18.776
2197	N	SER	888	28.604	74.242	17.558
2198	CA	SER	888	27.445	75.073	17.258
2199	HN	SER	888	28.899	74.133	18.507
2200	C	SER	888	26.109	74.426	16.874
2201	O	SER	888	25.280	75.109	16.273
2202	CB	SER	888	27.808	76.071	16.151
2203	OG	SER	888	28.887	76.954	16.451
2204	HG	SER	888	29.184	77.309	15.605
2205	N	VAL	889	25.838	73.039	17.163
2206	CA	VAL	889	24.556	72.431	16.670
2207	HN	VAL	889	26.322	72.541	17.906
2208	C	VAL	889	23.593	72.412	17.909
2209	O	VAL	889	23.913	71.900	18.962
2210	CB	VAL	889	24.621	71.056	15.955
2211	CG1	VAL	889	25.677	71.023	14.826
2212	CG2	VAL	889	24.864	69.889	16.914
2213	N	ASP	890	22.347	73.037	17.745
2214	CA	ASP	890	21.379	73.348	18.812
2215	HN	ASP	890	22.029	72.987	16.798
2216	C	ASP	890	20.246	72.324	19.082
2217	O	ASP	890	19.542	71.921	18.159
2218	CB	ASP	890	20.820	74.764	18.514
2219	CG	ASP	890	21.278	75.896	19.445
2220	OD1	ASP	890	22.383	76.413	19.372
2221	OD2	ASP	890	20.313	76.270	20.338
2222	HD2	ASP	890	20.643	76.966	20.885
2223	N	PHE	891	20.127	72.032	20.451
2224	CA	PHE	891	19.184	71.088	21.009
2225	HN	PHE	891	20.797	72.434	21.092
2226	C	PHE	891	17.936	71.983	21.374
2227	O	PHE	891	18.086	73.118	21.814
2228	CB	PHE	891	19.814	70.282	22.175
2229	CG	PHE	891	21.021	69.477	21.682
2230	CD1	PHE	891	20.987	68.025	21.698
2231	CE1	PHE	891	22.129	67.235	21.275
2232	CZ	PHE	891	23.323	67.884	20.817
2233	CE2	PHE	891	23.373	69.314	20.772
2234	CD2	PHE	891	22.247	70.111	21.206
2235	N	PRO	892	16.645	71.447	21.085
2236	CA	PRO	892	15.369	72.021	21.537
2237	CD	PRO	892	16.431	70.128	20.505
2238	C	PRO	892	15.213	71.856	23.072
2239	O	PRO	892	15.924	71.125	23.735
2240	CB	PRO	892	14.305	71.131	20.920
2241	CG	PRO	892	14.995	69.761	20.823
2242	N	GLU	893	14.098	72.520	23.629
2243	CA	GLU	893	13.795	72.507	25.059
2244	HN	GLU	893	13.417	72.885	22.994
2245	C	GLU	893	13.842	71.099	25.612
2246	O	GLU	893	14.651	70.779	26.492
2247	CB	GLU	893	12.399	73.087	25.305

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2248	CG	GLU	893	12.359	74.589	25.235
2249	CD	GLU	893	13.300	75.215	26.243
2250	OE1	GLU	893	14.507	74.896	26.220
2251	OE2	GLU	893	12.832	76.021	27.067
2252	HE2	GLU	893	13.523	76.332	27.631
2253	N	MET	894	12.947	70.271	25.087
2254	CA	MET	894	12.861	68.895	25.507
2255	HN	MET	894	12.320	70.609	24.386
2256	C	MET	894	14.249	68.252	25.562
2257	O	MET	894	14.870	68.271	26.618
2258	CB	MET	894	11.912	68.116	24.584
2259	CG	MET	894	10.604	67.677	25.273
2260	SD	MET	894	10.728	67.416	27.096
2261	CE	MET	894	11.156	65.740	27.227
2262	N	MET	895	14.844	67.682	24.391
2263	CA	MET	895	16.108	66.917	24.435
2264	HN	MET	895	14.463	67.895	23.478
2265	C	MET	895	17.168	67.650	25.267
2266	O	MET	895	17.989	66.999	25.886
2267	CB	MET	895	16.757	66.650	23.073
2268	CG	MET	895	15.965	65.699	22.172
2269	SD	MET	895	16.747	65.346	20.554
2270	CE	MET	895	18.397	66.112	20.684
2271	N	ALA	896	17.158	69.058	25.252
2272	CA	ALA	896	18.176	69.798	25.976
2273	HN	ALA	896	16.441	69.553	24.759
2274	C	ALA	896	18.197	69.481	27.480
2275	O	ALA	896	19.277	69.320	28.049
2276	CB	ALA	896	17.986	71.297	25.751
2277	N	GLU	897	17.013	69.378	28.106
2278	CA	GLU	897	16.852	69.103	29.554
2279	HN	GLU	897	16.185	69.496	27.559
2280	C	GLU	897	17.169	67.641	29.921
2281	O	GLU	897	17.828	67.362	30.929
2282	CB	GLU	897	15.399	69.460	30.000
2283	CG	GLU	897	15.155	69.773	31.529
2284	CD	GLU	897	14.687	71.232	31.813
2285	OE1	GLU	897	15.306	72.174	31.267
2286	OE2	GLU	897	13.718	71.441	32.590
2287	HE2	GLU	897	13.561	72.371	32.656
2288	N	ILE	898	16.693	66.718	29.088
2289	CA	ILE	898	16.906	65.293	29.296
2290	HN	ILE	898	16.168	67.015	28.290
2291	C	ILE	898	18.372	64.971	29.082
2292	O	ILE	898	18.963	64.230	29.866
2293	CB	ILE	898	16.065	64.484	28.325
2294	CG2	ILE	898	16.032	63.034	28.734
2295	CG1	ILE	898	14.641	65.010	28.340
2296	CD1	ILE	898	13.785	64.322	27.349
2297	N	ILE	899	19.013	65.460	27.911
2298	CA	ILE	899	20.391	65.025	27.815
2299	HN	ILE	899	18.613	66.102	27.232
2300	C	ILE	899	21.065	65.586	29.109
2301	O	ILE	899	21.557	64.777	29.867
2302	CB	ILE	899	21.118	65.405	26.543

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2303	CG2	ILE	899	22.558	64.893	26.717
2304	CG1	ILE	899	20.440	64.810	25.285
2305	CD1	ILE	899	20.622	65.767	24.106
2306	N	SER	900	21.002	67.001	29.398
2307	CA	SER	900	21.566	67.613	30.614
2308	HN	SER	900	20.553	67.602	28.736
2309	C	SER	900	21.374	66.795	31.884
2310	O	SER	900	22.286	66.672	32.706
2311	CB	SER	900	20.953	69.029	30.750
2312	OG	SER	900	19.545	69.053	30.493
2313	HG	SER	900	19.415	68.789	29.578
2314	N	VAL	901	20.169	66.272	32.061
2315	CA	VAL	901	19.888	65.470	33.231
2316	HN	VAL	901	19.451	66.433	31.384
2317	C	VAL	901	20.678	64.169	33.202
2318	O	VAL	901	21.380	63.839	34.153
2319	CB	VAL	901	18.336	65.184	33.317
2320	CG1	VAL	901	17.897	64.050	34.284
2321	CG2	VAL	901	17.492	66.416	33.722
2322	N	GLN	902	20.582	63.445	32.093
2323	CA	GLN	902	21.263	62.164	31.955
2324	HN	GLN	902	20.028	63.787	31.334
2325	C	GLN	902	22.784	62.163	31.856
2326	O	GLN	902	23.421	61.208	32.299
2327	CB	GLN	902	20.717	61.415	30.737
2328	CG	GLN	902	19.252	61.040	30.828
2329	CD	GLN	902	18.940	60.208	32.056
2330	OE1	GLN	902	19.638	59.237	32.361
2331	NE2	GLN	902	18.007	60.708	32.969
2332	1HE2	GLN	902	17.720	60.104	33.720
2333	2HE2	GLN	902	17.531	61.588	32.810
2334	N	VAL	903	23.371	63.214	31.288
2335	CA	VAL	903	24.819	63.244	31.093
2336	HN	VAL	903	22.815	63.991	30.991
2337	C	VAL	903	25.674	62.568	32.174
2338	O	VAL	903	26.442	61.655	31.866
2339	CB	VAL	903	25.318	64.719	30.822
2340	CG1	VAL	903	24.613	65.484	29.668
2341	CG2	VAL	903	25.217	65.652	32.053
2342	N	PRO	904	25.556	62.991	33.449
2343	CA	PRO	904	25.556	62.991	33.449
2344	CD	PRO	904	26.383	62.331	34.468
2345	C	PRO	904	24.668	63.995	34.066
2346	O	PRO	904	26.046	60.853	34.659
2347	CB	PRO	904	26.772	59.978	34.194
2348	CG	PRO	904	26.109	63.164	35.722
2349	N	LYS	905	24.691	63.591	35.528
2350	CA	LYS	905	24.927	60.589	35.323
2351	HN	LYS	905	24.462	59.233	35.620
2352	C	LYS	905	24.371	61.358	35.638
2353	O	LYS	905	24.605	58.128	34.550
2354	CB	LYS	905	24.720	56.946	34.900
2355	CG	LYS	905	22.996	59.291	36.064
2356	CD	LYS	905	22.030	59.560	34.928
2357	CE	LYS	905	20.583	59.336	35.345
				20.083	60.442	36.262

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2358	NZ	LYS	905	18.618	60.349	36.653
2359	HZ1	LYS	905	18.227	61.297	36.749
2360	HZ2	LYS	905	18.100	59.837	35.925
2361	HZ3	LYS	905	18.535	59.864	37.523
2362	N	ILE	906	24.590	58.493	33.265
2363	CA	ILE	906	24.699	57.512	32.172
2364	HN	ILE	906	24.502	59.463	33.038
2365	C	ILE	906	26.087	56.939	31.960
2366	O	ILE	906	26.376	55.800	32.329
2367	CB	ILE	906	24.127	58.174	30.852
2368	CG1	ILE	906	22.814	57.521	30.312
2369	CG2	ILE	906	25.168	58.202	29.690
2370	CD1	ILE	906	21.527	58.350	30.491
2371	N	LEU	907	26.923	57.761	31.330
2372	CA	LEU	907	28.298	57.423	30.985
2373	HN	LEU	907	26.586	58.668	31.076
2374	C	LEU	907	28.968	56.365	31.867
2375	O	LEU	907	29.557	55.412	31.351
2376	CB	LEU	907	29.155	58.720	30.925
2377	CG	LEU	907	29.319	59.549	32.227
2378	CD1	LEU	907	30.099	60.838	31.937
2379	CD2	LEU	907	27.973	59.894	32.885
2380	N	SER	908	28.866	56.524	33.185
2381	CA	SER	908	29.473	55.585	34.132
2382	HN	SER	908	28.358	57.309	33.540
2383	C	SER	908	28.974	54.145	33.984
2384	O	SER	908	29.703	53.261	33.522
2385	CB	SER	908	29.242	56.123	35.566
2386	OG	SER	908	28.881	57.509	35.589
2387	HG	SER	908	29.621	58.005	35.229
2388	N	GLY	909	27.727	53.925	34.405
2389	CA	GLY	909	27.115	52.605	34.341
2390	HN	GLY	909	27.198	54.688	34.776
2391	C	GLY	909	26.426	52.237	35.647
2392	O	GLY	909	26.387	51.071	36.044
2393	N	LYS	910	25.865	53.251	36.308
2394	CA	LYS	910	25.182	53.106	37.593
2395	HN	LYS	910	25.915	54.163	35.901
2396	C	LYS	910	23.655	52.955	37.392
2397	O	LYS	910	22.850	53.294	38.269
2398	CB	LYS	910	25.508	54.360	38.450
2399	CG	LYS	910	26.794	55.097	37.998
2400	CD	LYS	910	26.636	56.607	37.803
2401	CE	LYS	910	27.995	57.214	37.429
2402	NZ	LYS	910	27.817	58.633	37.073
2403	HZ2	LYS	910	27.105	59.070	37.670
2404	HZ1	LYS	910	28.680	59.166	37.222
2405	HZ3	LYS	910	27.542	58.704	36.114
2406	N	VAL	911	23.302	52.427	36.214
2407	CA	VAL	911	21.929	52.172	35.734
2408	HN	VAL	911	24.046	52.179	35.594
2409	C	VAL	911	21.828	50.671	35.391
2410	O	VAL	911	22.809	50.084	34.932
2411	CB	VAL	911	21.666	53.060	34.454
2412	CG1	VAL	911	21.087	54.480	34.706

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2413	CG2	VAL	911	22.921	53.281	33.575
2414	N	LYS	912	20.666	50.053	35.581
2415	CA	LYS	912	20.552	48.628	35.274
2416	HN	LYS	912	19.877	50.558	35.931
2417	C	LYS	912	19.777	48.267	34.014
2418	O	LYS	912	18.544	48.228	34.010
2419	CB	LYS	912	19.948	47.873	36.448
2420	CG	LYS	912	19.772	46.377	36.216
2421	CD	LYS	912	18.912	45.841	37.339
2422	CE	LYS	912	18.472	44.409	37.153
2423	NZ	LYS	912	17.517	43.918	38.231
2424	HZ1	LYS	912	16.988	44.716	38.611
2425	HZ2	LYS	912	16.862	43.235	37.825
2426	HZ3	LYS	912	18.038	43.483	38.965
2427	N	PRO	913	20.528	47.980	32.960
2428	CA	PRO	913	19.971	47.592	31.674
2429	C	PRO	913	19.437	46.168	31.795
2430	O	PRO	913	20.208	45.247	32.038
2431	CB	PRO	913	21.081	47.729	30.622
2432	CG	PRO	913	22.370	47.474	31.418
2433	CD	PRO	913	22.090	48.144	32.766
2434	N	ILE	914	18.132	45.976	31.641
2435	CA	ILE	914	17.573	44.628	31.718
2436	HN	ILE	914	17.529	46.756	31.472
2437	C	ILE	914	17.956	43.896	30.438
2438	O	ILE	914	17.995	44.499	29.370
2439	CB	ILE	914	16.003	44.733	31.889
2440	CG1	ILE	914	15.530	45.812	32.915
2441	CG2	ILE	914	15.345	43.373	32.279
2442	CD1	ILE	914	14.007	45.901	33.144
2443	N	TYR	915	18.239	42.605	30.527
2444	CA	TYR	915	18.602	41.856	29.326
2445	HN	TYR	915	18.204	42.144	31.413
2446	C	TYR	915	17.790	40.570	29.208
2447	O	TYR	915	17.364	40.025	30.218
2448	CB	TYR	915	20.110	41.472	29.342
2449	CG	TYR	915	21.114	42.616	29.160
2450	CD1	TYR	915	22.470	42.349	28.948
2451	CD2	TYR	915	20.670	43.942	29.198
2452	CE1	TYR	915	23.368	43.398	28.768
2453	CE2	TYR	915	21.570	44.988	29.019
2454	CZ	TYR	915	22.919	44.715	28.804
2455	OH	TYR	915	23.803	45.741	28.625
2456	HH	TYR	915	23.322	46.569	28.679
2457	N	PHE	916	17.547	40.099	27.984
2458	CA	PHE	916	16.801	38.847	27.812
2459	HN	PHE	916	17.873	40.599	27.182
2460	C	PHE	916	17.772	37.692	27.803
2461	O	PHE	916	17.483	36.618	28.320
2462	CB	PHE	916	16.012	38.831	26.509
2463	CG	PHE	916	14.782	39.658	26.558
2464	CD1	PHE	916	13.647	39.198	27.206
2465	CE1	PHE	916	12.534	40.005	27.331
2466	CZ	PHE	916	12.552	41.283	26.807
2467	CE2	PHE	916	13.680	41.743	26.155

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2468	CD2	PHE	916	14.787	40.933	26.035
2469	N	HIS	917	18.929	37.930	27.198
2470	CA	HIS	917	19.985	36.938	27.104
2471	HN	HIS	917	19.079	38.830	26.789
2472	C	HIS	917	21.218	37.571	27.755
2473	O	HIS	917	21.857	38.430	27.144
2474	OXT	HIS	917	22.578	37.226	28.030
2475	CB	HIS	917	20.300	36.628	25.631
2476	CG	HIS	917	19.093	36.359	24.792
2477	ND1	HIS	917	18.208	35.328	25.058
2478	CE1	HIS	917	17.249	35.325	24.154
2479	NE2	HIS	917	17.471	36.322	23.306
2480	CD2	HIS	917	18.612	36.976	23.686
2481	HE2	HIS	917	16.900	36.556	22.520
2482	N1	BIC	1	13.946	58.376	15.059
2483	C2	BIC	1	14.799	59.044	15.463
2484	C3	BIC	1	15.841	59.881	15.953
2485	C4	BIC	1	15.755	61.284	15.720
2486	C5	BIC	1	14.563	61.950	15.018
2487	F6	BIC	1	13.473	61.888	15.833
2488	F7	BIC	1	14.284	61.324	13.839
2489	F8	BIC	1	14.827	63.259	14.743
2490	C9	BIC	1	16.847	62.050	16.204
2491	C10	BIC	1	17.942	61.475	16.889
2492	N11	BIC	1	18.989	62.358	17.280
2493	C12	BIC	1	20.087	62.115	18.161
2494	O13	BIC	1	20.203	61.135	18.877
2495	C14	BIC	1	21.226	63.177	18.098
2496	C15	BIC	1	20.663	64.593	18.310
2497	O16	BIC	1	22.231	62.983	19.086
2498	C17	BIC	1	21.912	63.056	16.727
2499	S18	BIC	1	22.550	61.414	16.461
2500	O19	BIC	1	23.652	61.024	17.469
2501	O20	BIC	1	21.445	60.344	16.394
2502	C21	BIC	1	23.155	61.723	14.866
2503	C22	BIC	1	22.265	61.621	13.774
2504	C23	BIC	1	22.764	61.780	12.465
2505	C24	BIC	1	24.122	62.129	12.302
2506	F25	BIC	1	24.627	62.319	11.037
2507	C26	BIC	1	24.991	62.301	13.395
2508	C27	BIC	1	24.507	62.085	14.702
2509	C28	BIC	1	17.982	60.076	17.127
2510	C29	BIC	1	16.918	59.274	16.650
2511	H33	BIC	1	18.992	63.281	16.873
2512	H39	BIC	1	22.378	62.027	19.128

TABLE 5

ATOMIC COORDINATES OF PR IN COMPLEX WITH RWJ-60130
OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL
STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP

Atom Number	Atom Symbol	Residue Name	Residue Number	X Coordinate	Y Coordinate	Z Coordinate
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1	N	GLN	682	-15.010	41.258	15.638
2	HN1	GLN	682	-15.045	42.257	15.389
3	HN2	GLN	682	-14.426	40.755	14.955
4	CA	GLN	682	-14.439	41.109	16.970
5	C	GLN	682	-14.873	42.160	18.025
6	O	GLN	682	-15.047	41.805	19.197
7	CB	GLN	682	-12.914	41.005	16.866
8	CG	GLN	682	-12.305	41.836	15.765
9	CD	GLN	682	-12.397	43.302	16.071
10	OE1	GLN	682	-12.505	43.688	17.231
11	NE2	GLN	682	-12.345	44.181	14.969
12	1HE2	GLN	682	-12.352	45.177	15.141
13	2HE2	GLN	682	-12.214	43.835	14.031
14	HN3	GLN	682	-15.936	40.879	15.627
15	N	LEU	683	-15.080	43.419	17.608
16	CA	LEU	683	-15.510	44.539	18.490
17	HN	LEU	683	-14.935	43.618	16.639
18	C	LEU	683	-15.065	44.431	19.944
19	O	LEU	683	-15.839	44.716	20.859
20	CB	LEU	683	-17.038	44.695	18.484
21	CG	LEU	683	-17.799	45.363	17.338
22	CD1	LEU	683	-17.383	44.762	16.011
23	CD2	LEU	683	-19.300	45.185	17.568
24	N	ILE	684	-13.816	44.047	20.146
25	CA	ILE	684	-13.270	43.859	21.478
26	HN	ILE	684	-13.227	43.881	19.355
27	C	ILE	684	-11.755	44.117	21.381
28	O	ILE	684	-11.026	43.391	20.698
29	CB	ILE	684	-13.587	42.385	21.960
30	CG1	ILE	684	-13.414	42.151	23.496
31	CG2	ILE	684	-12.746	41.308	21.208
32	CD1	ILE	684	-14.014	40.842	24.049
33	N	PRO	685	-11.269	45.167	22.062
34	CA	PRO	685	-9.856	45.563	22.059
35	CD	PRO	685	-11.987	45.849	23.154
36	C	PRO	685	-8.881	44.516	22.556
37	O	PRO	685	-9.106	43.879	23.581
38	CB	PRO	685	-9.853	46.799	22.947
39	CG	PRO	685	-10.854	46.430	23.987
40	N	PRO	686	-7.801	44.333	21.810
41	CA	PRO	686	-6.772	43.402	22.220
42	C	PRO	686	-5.691	44.331	22.701
43	O	PRO	686	-5.692	45.515	22.363
44	CB	PRO	686	-6.319	42.505	21.059
45	CG	PRO	686	-6.674	43.324	19.808
46	CD	PRO	686	-8.000	43.988	20.187
47	N	LEU	687	-4.769	43.820	23.494
48	CA	LEU	687	-3.723	44.678	24.008
49	HN	LEU	687	-4.792	42.851	23.738
50	C	LEU	687	-2.861	45.295	22.900
51	O	LEU	687	-2.512	46.478	22.951
52	CB	LEU	687	-2.879	43.883	24.978
53	CG	LEU	687	-1.894	44.651	25.842
54	CD1	LEU	687	-2.286	46.117	26.083
55	CD2	LEU	687	-1.842	43.877	27.129

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56	N	ILE	688	-2.521	44.494	21.898
57	CA	ILE	688	-1.721	44.978	20.786
58	HN	ILE	688	-2.821	43.540	21.909
59	C	ILE	688	-2.621	45.837	19.898
60	O	ILE	688	-2.148	46.601	19.056
61	CB	ILE	688	-1.130	43.737	20.000
62	CG1	ILE	688	-2.201	42.834	19.307
63	CG2	ILE	688	-0.234	42.826	20.895
64	CD1	ILE	688	-1.662	41.818	18.279
65	N	ASN	689	-3.931	45.693	20.088
66	CA	ASN	689	-4.913	46.442	19.306
67	HN	ASN	689	-4.252	45.054	20.786
68	C	ASN	689	-4.859	47.910	19.668
69	O	ASN	689	-4.889	48.806	18.829
70	CB	ASN	689	-6.326	45.855	19.591
71	CG	ASN	689	-7.519	46.578	18.956
72	OD1	ASN	689	-8.064	46.169	17.942
73	ND2	ASN	689	-7.952	47.680	19.507
74	IHD2	ASN	689	-8.644	48.160	18.925
75	2HD2	ASN	689	-7.420	48.042	20.298
76	N	LEU	690	-4.799	48.126	20.963
77	CA	LEU	690	-4.752	49.439	21.528
78	HN	LEU	690	-4.784	47.339	21.580
79	C	LEU	690	-3.362	50.002	21.308
80	O	LEU	690	-3.176	51.209	21.154
81	CB	LEU	690	-5.047	49.288	22.995
82	CG	LEU	690	-5.349	50.530	23.767
83	CD1	LEU	690	-6.690	50.364	24.404
84	CD2	LEU	690	-4.307	50.719	24.805
85	N	LEU	691	-2.374	49.119	21.292
86	CA	LEU	691	-1.001	49.552	21.090
87	HN	LEU	691	-2.574	48.147	21.419
88	C	LEU	691	-0.869	50.120	19.665
89	O	LEU	691	-0.131	51.073	19.421
90	CB	LEU	691	-0.068	48.363	21.316
91	CG	LEU	691	1.250	48.527	22.075
92	CD1	LEU	691	1.095	49.268	23.390
93	CD2	LEU	691	1.764	47.137	22.328
94	N	MET	692	1.764	49.544	18.727
95	CA	MET	692	-1.606	50.045	17.376
96	HN	MET	692	-1.547	48.770	18.954
97	C	MET	692	-2.197	51.347	17.200
98	O	MET	692	-2.330	52.246	16.524
99	CB	MET	692	-1.845	48.959	16.384
100	CG	MET	692	-2.049	49.409	14.916
101	SD	MET	692	-2.206	47.993	13.887
102	CE	MET	692	-2.628	48.850	12.317
103	N	SER	693	-2.810	51.484	17.797
104	CA	SER	693	-3.518	52.738	17.584
105	HN	SER	693	-4.251	50.756	18.370
106	C	SER	693	-3.895	53.964	18.253
107	O	SER	693	-3.645	55.082	17.931
108	CB	SER	693	-4.043	52.588	17.923
109	OG	SER	693	-5.755	51.270	17.670
110	HG	SER	693	-6.254	51.109	16.726

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111	N	ILE	694	-2.694	53.786	19.173
112	CA	ILE	694	-2.079	54.944	19.831
113	HN	ILE	694	-2.400	52.861	19.414
114	C	ILE	694	-0.672	55.231	19.325
115	O	ILE	694	0.069	56.001	19.939
116	CB	ILE	694	-1.980	54.783	21.367
117	CG2	ILE	694	-3.269	54.216	21.925
118	CG1	ILE	694	-0.801	53.879	21.725
119	CD1	ILE	694	-0.570	53.751	23.208
120	N	GLU	695	-0.301	54.606	18.214
121	CA	GLU	695	1.020	54.801	17.640
122	HN	GLU	695	-0.944	53.988	17.762
123	C	GLU	695	1.093	56.227	17.144
124	O	GLU	695	0.148	56.718	16.543
125	CB	GLU	695	1.238	53.825	16.483
126	CG	GLU	695	2.643	53.807	15.879
127	CD	GLU	695	3.760	53.831	16.920
128	OE1	GLU	695	3.570	53.258	18.018
129	OE2	GLU	695	4.832	54.413	16.631
130	HE2	GLU	695	5.431	54.352	17.360
131	N	PRO	696	2.175	56.936	17.458
132	CA	PRO	696	2.104	58.288	16.900
133	CD	PRO	696	2.935	56.915	18.715
134	C	PRO	696	2.205	58.244	15.379
135	O	PRO	696	2.532	57.209	14.789
136	CB	PRO	696	3.278	59.025	17.552
137	CG	PRO	696	3.904	58.034	18.527
138	N	ASP	697	1.909	59.358	14.734
139	CA	ASP	697	1.979	59.373	13.291
140	HN	ASP	697	1.640	60.179	15.237
141	C	ASP	697	3.198	60.165	12.862
142	O	ASP	697	3.578	61.123	13.536
143	CB	ASP	697	0.666	59.986	12.735
144	CG	ASP	697	0.355	61.433	13.143
145	OD1	ASP	697	-0.395	62.158	12.506
146	OD2	ASP	697	0.984	61.806	14.298
147	HD2	ASP	697	0.761	62.700	14.504
148	N	VAL	698	3.807	59.769	11.747
149	CA	VAL	698	5.012	60.440	11.267
150	HN	VAL	698	3.433	58.999	11.229
151	C	VAL	698	4.883	61.937	11.156
152	O	VAL	698	3.915	62.458	10.611
153	CB	VAL	698	5.466	59.926	9.887
154	CG1	VAL	698	5.970	58.504	10.001
155	CG2	VAL	698	4.322	60.031	8.885
156	N	ILE	699	5.876	62.639	11.673
157	CA	ILE	699	5.854	64.080	11.590
158	HN	ILE	699	6.640	62.174	12.120
159	C	ILE	699	7.097	64.568	10.856
160	O	ILE	699	8.225	64.160	11.169
161	CB	ILE	699	5.736	64.714	13.036
162	CG1	ILE	699	6.895	64.330	14.012
163	CG2	ILE	699	4.383	64.379	13.735
164	CD1	ILE	699	6.826	64.960	15.418
165	N	TYR	700	6.859	65.427	9.863

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166	CA	TYR	700	7.899	65.995	9.007
167	HN	TYR	700	5.912	65.698	9.695
168	C	TYR	700	8.844	66.938	9.690
169	O	TYR	700	8.559	67.480	10.759
170	CB	TYR	700	7.285	66.703	7.797
171	CG	TYR	700	6.627	65.742	6.847
172	CD1	TYR	700	5.329	65.966	6.401
173	CE1	TYR	700	4.665	65.026	5.623
174	CZ	TYR	700	5.300	63.843	5.279
175	OH	TYR	700	4.635	62.900	4.526
176	HH	TYR	700	5.069	62.049	4.659
177	CE2	TYR	700	6.608	63.600	5.697
178	CD2	TYR	700	7.262	64.551	6.478
179	N	ALA	701	9.971	67.152	9.023
180	CA	ALA	701	11.029	67.995	9.539
181	HN	ALA	701	10.094	66.714	8.133
182	C	ALA	701	10.957	69.476	9.185
183	O	ALA	701	11.645	70.282	9.806
184	CB	ALA	701	12.359	67.437	9.100
185	N	GLY	702	10.142	69.846	8.202
186	CA	GLY	702	10.071	71.249	7.828
187	HN	GLY	702	9.584	69.167	7.725
188	C	GLY	702	11.445	71.762	7.423
189	O	GLY	702	11.889	72.816	7.879
190	N	HIS	703	12.131	71.003	6.571
191	CA	HIS	703	13.464	71.376	6.102
192	HN	HIS	703	11.722	70.153	6.241
193	C	HIS	703	13.342	72.135	4.797
194	O	HIS	703	12.377	71.977	4.040
195	CB	HIS	703	14.316	70.111	5.907
196	CG	HIS	703	15.770	70.427	5.713
197	ND1	HIS	703	16.648	70.863	6.702
198	CE1	HIS	703	17.810	70.793	6.025
199	NE2	HIS	703	17.774	70.374	4.731
200	CD2	HIS	703	16.439	70.135	4.532
201	HE2	HIS	703	18.550	70.259	4.064
202	N	ASP	704	14.333	72.973	4.559
203	CA	ASP	704	14.410	73.739	3.341
204	HN	ASP	704	15.053	73.080	5.244
205	C	ASP	704	15.539	73.046	2.609
206	O	ASP	704	16.712	73.253	2.928
207	CB	ASP	704	14.801	75.179	3.628
208	CG	ASP	704	14.786	76.022	2.386
209	OD1	ASP	704	14.680	75.431	1.294
210	OD2	ASP	704	14.881	77.259	2.497
211	HD2	ASP	704	14.858	77.655	1.639
212	N	ASN	705	15.184	72.196	1.658
213	CA	ASN	705	16.169	71.457	0.886
214	HN	ASN	705	14.212	72.058	1.467
215	C	ASN	705	16.414	72.208	-0.411
216	O	ASN	705	17.014	71.684	-1.351
217	CB	ASN	705	15.643	70.020	0.600
218	CG	ASN	705	14.332	69.904	-0.185
219	OD1	ASN	705	14.308	69.649	-1.380
220	ND2	ASN	705	13.204	70.107	0.440

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221	1HD2	ASN	705	12.407	70.157	-0.200
222	2HD2	ASN	705	13.262	70.406	1.414
223	N	THR	706	15.935	73.449	-0.435
224	CA	THR	706	16.057	74.325	-1.592
225	HN	THR	706	15.470	73.797	0.379
226	C	THR	706	17.406	74.995	-1.581
227	O	THR	706	17.708	75.846	-2.418
228	CB	THR	706	14.910	75.390	-1.546
229	OG1	THR	706	15.333	76.547	-0.837
230	HG1	THR	706	14.613	77.181	-0.907
231	CG2	THR	706	13.605	74.960	-0.840
232	N	LYS	707	18.223	74.651	-0.605
233	CA	LYS	707	19.517	75.267	-0.548
234	HN	LYS	707	17.947	73.976	0.079
235	C	LYS	707	20.441	74.218	0.032
236	O	LYS	707	20.052	73.480	0.945
237	CB	LYS	707	19.445	76.516	0.374
238	CG	LYS	707	18.097	77.274	0.280
239	CD	LYS	707	18.015	78.548	1.126
240	CE	LYS	707	16.663	79.230	0.883
241	NZ	LYS	707	16.507	80.357	1.819
242	HZ2	LYS	707	17.405	80.833	1.966
243	HZ1	LYS	707	15.867	81.066	1.446
244	HZ3	LYS	707	16.158	80.019	2.693
245	N	PRO	708	21.688	74.161	-0.473
246	CA	PRO	708	22.654	73.163	-0.016
247	CD	PRO	708	22.365	75.246	-1.206
248	C	PRO	708	22.661	72.720	1.398
249	O	PRO	708	22.222	73.405	2.316
250	CB	PRO	708	24.018	73.697	-0.465
251	CG	PRO	708	23.812	75.102	-0.777
252	N	ASP	709	23.175	71.516	1.550
253	CA	ASP	709	23.249	70.949	2.849
254	HN	ASP	709	23.511	71.006	0.757
255	C	ASP	709	24.550	71.260	3.463
256	O	ASP	709	25.441	71.872	2.877
257	CB	ASP	709	23.091	69.450	2.784
258	CG	ASP	709	21.834	69.063	2.108
259	OD1	ASP	709	20.895	69.889	2.139
260	OD2	ASP	709	21.777	67.951	1.553
261	HD2	ASP	709	20.924	67.836	1.164
262	N	THR	710	24.636	70.819	4.690
263	CA	THR	710	25.823	70.973	5.447
264	HN	THR	710	23.847	70.365	5.104
265	C	THR	710	25.383	70.258	6.675
266	O	THR	710	24.204	70.267	7.041
267	CB	THR	710	26.132	72.475	5.761
268	OG1	THR	710	25.356	72.923	6.865
269	HG1	THR	710	25.645	73.822	7.048
270	CG2	THR	710	25.824	73.487	4.637
271	N	SER	711	26.329	69.578	7.289
272	CA	SER	711	25.985	68.820	8.444
273	HN	SER	711	27.270	69.593	6.950
274	C	SER	711	25.348	69.652	9.408
275	O	SER	711	24.169	69.484	9.541

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				27.252	68.144	9.023
276	CB	SER	711	28.080	67.556	8.013
277	OG	SER	711	27.569	66.859	7.593
278	HG	SER	711	26.114	70.494	10.112
279	N	SER	712	25.527	71.392	11.074
280	CA	SER	712	27.104	70.500	9.969
281	HN	SER	712	24.166	71.500	10.449
282	C	SER	712	23.511	70.508	10.391
283	O	SER	712	26.267	72.753	11.066
284	CB	SER	712	27.583	72.674	11.625
285	OG	SER	712	27.489	72.421	12.547
286	HG	SER	712	23.678	72.598	9.944
287	N	SER	713	22.339	72.472	9.371
288	CA	SER	713	24.182	73.462	9.948
289	HN	SER	713	21.406	71.259	9.586
290	C	SER	713	20.256	71.418	9.959
291	O	SER	713	22.505	72.804	7.867
292	CB	SER	713	21.363	73.468	7.314
293	OG	SER	713	20.620	72.862	7.377
294	HG	SER	713	21.874	70.055	9.313
295	N	LEU	714	21.017	68.898	9.427
296	CA	LEU	714	22.826	69.943	9.027
297	HN	LEU	714	20.938	68.217	10.741
298	C	LEU	714	19.956	67.556	11.097
299	O	LEU	714	21.502	67.918	8.321
300	CB	LEU	714	21.248	68.304	6.839
301	CG	LEU	714	21.363	67.062	5.943
302	CD1	LEU	714	19.880	68.972	6.625
303	CD2	LEU	714	22.058	68.261	11.408
304	N	LEU	715	22.089	67.687	12.697
305	CA	LEU	715	22.873	68.690	11.016
306	HN	LEU	715	21.204	68.642	13.356
307	C	LEU	715	20.386	68.325	14.216
308	O	LEU	715	23.540	67.807	13.243
309	CB	LEU	715	24.610	66.823	12.697
310	CG	LEU	715	25.926	66.993	13.467
311	CD1	LEU	715	24.157	65.355	12.764
312	CD2	LEU	715	21.348	69.874	12.942
313	N	THR	716	20.571	70.736	13.707
314	CA	THR	716	21.934	70.157	12.182
315	HN	THR	716	19.114	70.479	13.542
316	C	THR	716	18.437	70.227	14.534
317	O	THR	716	20.967	72.126	13.506
318	CB	THR	716	21.793	72.724	14.509
319	OG1	THR	716	22.011	73.607	14.181
320	HG1	THR	716	19.768	72.979	13.458
321	CG2	THR	716	18.638	70.483	12.305
322	N	SER	717	17.243	70.208	12.067
323	CA	SER	717	19.248	70.677	11.536
324	HN	SER	717	16.872	68.910	12.817
325	C	SER	717	15.856	68.912	13.493
326	O	SER	717	16.926	70.103	10.554
327	CB	SER	717	17.601	69.011	9.919
328	OG	SER	717	18.545	69.178	9.987
329	HG	SER	717	17.691	67.844	12.756
330	N	LEU	718			

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331	CA	LEU	718	17.371	66.544	13.424
332	HN	LEU	718	18.546	67.924	12.244
333	C	LEU	718	17.026	66.582	14.903
334	O	LEU	718	16.107	65.898	15.360
335	CB	LEU	718	18.454	65.464	13.111
336	CG	LEU	718	17.916	64.771	11.843
337	CD1	LEU	718	16.946	65.767	11.273
338	CD2	LEU	718	18.930	64.423	10.767
339	N	ASN	719	17.745	67.412	15.634
340	CA	ASN	719	17.523	67.628	17.058
341	HN	ASN	719	18.481	67.921	15.188
342	C	ASN	719	16.166	68.279	17.320
343	O	ASN	719	15.458	67.918	18.260
344	CB	ASN	719	18.614	68.525	17.580
345	CG	ASN	719	19.895	67.790	17.829
346	OD1	ASN	719	20.167	66.736	17.265
347	ND2	ASN	719	20.913	68.674	18.216
348	1HD2	ASN	719	21.861	68.327	18.261
349	2HD2	ASN	719	20.709	69.592	18.580
350	N	GLN	720	15.824	69.277	16.515
351	CA	GLN	720	14.531	69.918	16.671
352	HN	GLN	720	16.455	69.586	15.803
353	C	GLN	720	13.553	68.764	16.493
354	O	GLN	720	12.674	68.521	17.327
355	CB	GLN	720	14.336	70.984	15.571
356	CG	GLN	720	14.185	72.462	16.060
357	CD	GLN	720	15.330	73.109	16.849
358	OE1	GLN	720	15.113	73.748	17.867
359	NE2	GLN	720	16.562	73.003	16.420
360	2HE2	GLN	720	16.667	72.516	15.528
361	1HE2	GLN	720	17.255	73.517	16.966
362	N	LEU	721	13.738	68.029	15.402
363	CA	LEU	721	12.865	66.914	15.121
364	HN	LEU	721	14.483	68.250	14.773
365	C	LEU	721	12.721	65.969	16.297
366	O	LEU	721	11.628	65.467	16.561
367	CB	LEU	721	13.353	66.111	13.921
368	CG	LEU	721	12.281	65.040	13.743
369	CD1	LEU	721	10.943	65.750	13.669
370	CD2	LEU	721	12.512	64.192	12.523
371	N	GLY	722	13.828	65.713	16.988
372	CA	GLY	722	13.811	64.809	18.123
373	HN	GLY	722	14.687	66.151	16.721
374	C	GLY	722	12.951	65.353	19.242
375	O	GLY	722	12.220	64.609	19.904
376	N	GLU	723	13.057	66.663	19.443
377	CA	GLU	723	12.278	67.325	20.462
378	HN	GLU	723	13.687	67.198	18.879
379	C	GLU	723	10.824	67.093	20.146
380	O	GLU	723	10.057	66.625	20.979
381	CB	GLU	723	12.612	68.843	20.496
382	CG	GLU	723	12.287	69.677	19.213
383	CD	GLU	723	12.698	71.151	19.181
384	OE1	GLU	723	12.514	71.873	18.210
385	OE2	GLU	723	13.285	71.582	20.332

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386	HE2	GLU	723	13.514	72.495	20.248
387	N	ARG	724	10.411	67.381	18.930
388	CA	ARG	724	9.016	67.165	18.680
389	HN	ARG	724	11.031	67.728	18.226
390	C	ARG	724	8.576	65.706	18.864
391	O	ARG	724	7.454	65.462	19.302
392	CB	ARG	724	8.675	67.723	17.311
393	CG	ARG	724	9.113	69.186	17.218
394	CD	ARG	724	8.843	69.724	15.849
395	NE	ARG	724	7.501	69.334	15.445
396	CZ	ARG	724	7.222	68.779	14.275
397	NH1	ARG	724	8.173	68.495	13.340
398	1HH1	ARG	724	7.915	68.079	12.463
399	2HH1	ARG	724	9.132	68.701	13.519
400	NH2	ARG	724	5.922	68.492	13.989
401	1HH2	ARG	724	5.691	68.079	13.109
402	2HH2	ARG	724	5.210	68.697	14.659
403	HE	ARG	724	6.750	69.494	16.085
404	N	GLN	725	9.468	64.745	18.588
405	CA	GLN	725	9.152	63.311	18.716
406	HN	GLN	725	10.383	65.011	18.284
407	C	GLN	725	9.183	62.733	20.124
408	O	GLN	725	8.499	61.746	20.406
409	CB	GLN	725	10.104	62.471	17.867
410	CG	GLN	725	9.763	62.367	16.396
411	CD	GLN	725	10.923	61.811	15.594
412	OE1	GLN	725	10.753	61.361	14.460
413	NE2	GLN	725	12.140	61.680	16.282
414	1HE2	GLN	725	12.859	61.134	15.843
415	2HE2	GLN	725	12.241	61.966	17.241
416	N	LEU	726	10.009	63.314	20.993
417	CA	LEU	726	10.114	62.841	22.369
418	HN	LEU	726	10.568	64.088	20.697
419	C	LEU	726	8.899	63.352	23.142
420	O	LEU	726	8.473	62.756	24.139
421	CB	LEU	726	11.436	63.328	23.029
422	CG	LEU	726	11.755	62.846	24.470
423	CD1	LEU	726	11.921	61.320	24.492
424	CD2	LEU	726	13.011	63.512	25.055
425	N	LEU	727	8.336	64.448	22.642
426	CA	LEU	727	7.145	65.049	23.218
427	HN	LEU	727	8.749	64.876	21.837
428	C	LEU	727	5.975	64.151	22.835
429	O	LEU	727	5.085	63.912	23.641
430	CB	LEU	727	6.932	66.496	22.689
431	CG	LEU	727	7.678	67.654	23.405
432	CD1	LEU	727	7.808	68.860	22.465
433	CD2	LEU	727	6.990	68.086	24.711
434	N	SER	728	5.988	63.628	21.616
435	CA	SER	728	4.923	62.724	21.198
436	HN	SER	728	6.728	63.855	20.983
437	C	SER	728	5.107	61.377	21.913
438	O	SER	728	4.165	60.573	22.006
439	CB	SER	728	4.957	62.561	19.658
440	OG	SER	728	6.142	61.904	19.194

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441	HG	SER	728	6.889	62.462	19.424
442	N	VAL	729	6.328	61.159	22.422
443	CA	VAL	729	6.726	59.930	23.143
444	HN	VAL	729	7.016	61.876	22.307
445	C	VAL	729	6.098	59.865	24.535
446	O	VAL	729	5.860	58.789	25.096
447	CB	VAL	729	8.302	59.869	23.233
448	CG1	VAL	729	8.899	58.734	24.111
449	CG2	VAL	729	9.004	59.734	21.860
450	N	VAL	730	5.853	61.042	25.092
451	CA	VAL	730	5.240	61.166	26.387
452	HN	VAL	730	6.103	61.873	24.594
453	C	VAL	730	3.724	60.950	26.214
454	O	VAL	730	3.127	60.223	27.013
455	CB	VAL	730	5.571	62.543	26.984
456	CG1	VAL	730	4.977	62.676	28.383
457	CG2	VAL	730	7.094	62.724	27.016
458	N	LYS	731	3.089	61.547	25.190
459	CA	LYS	731	1.644	61.294	25.014
460	HN	LYS	731	3.584	62.147	24.561
461	C	LYS	731	1.536	59.802	24.651
462	O	LYS	731	0.566	59.132	25.009
463	CB	LYS	731	0.963	62.138	23.883
464	CG	LYS	731	0.856	63.702	24.059
465	CD	LYS	731	-0.247	64.447	23.158
466	CE	LYS	731	-0.072	64.305	21.606
467	NZ	LYS	731	-0.903	65.223	20.724
468	HZ1	LYS	731	-0.504	66.173	20.744
469	HZ2	LYS	731	-0.896	64.870	19.757
470	HZ3	LYS	731	-1.844	65.249	21.061
471	N	TRP	732	2.523	59.265	23.943
472	CA	TRP	732	2.427	57.855	23.605
473	HN	TRP	732	3.307	59.813	23.652
474	C	TRP	732	2.531	57.001	24.873
475	O	TRP	732	1.647	56.190	25.144
476	CB	TRP	732	3.514	57.461	22.599
477	CG	TRP	732	3.692	55.982	22.458
478	CD1	TRP	732	2.865	55.102	21.832
479	NE1	TRP	732	3.387	53.831	21.906
480	CE2	TRP	732	4.576	53.879	22.585
481	CD2	TRP	732	4.778	55.221	22.976
482	HE1	TRP	732	2.967	53.007	21.526
483	CE3	TRP	732	5.938	55.547	23.688
484	CZ3	TRP	732	6.813	54.537	24.037
485	CH2	TRP	732	6.583	53.207	23.640
486	CZ2	TRP	732	5.459	52.858	22.937
487	N	SER	733	3.594	57.202	25.646
488	CA	SER	733	3.823	56.439	26.880
489	HN	SER	733	4.261	57.897	25.377
490	C	SER	733	2.603	56.421	27.797
491	O	SER	733	2.173	55.353	28.240
492	CB	SER	733	5.072	57.002	27.604
493	OG	SER	733	4.850	58.298	28.171
494	HG	SER	733	4.662	58.901	27.446
495	N	LYS	734	2.056	57.602	28.074

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496	CA	LYS	734	0.877	57.749	28.915
497	HN	LYS	734	2.473	58.425	27.688
498	C	LYS	734	-0.310	56.892	28.435
499	O	LYS	734	-1.087	56.394	29.246
500	CB	LYS	734	0.487	59.228	28.972
501	CG	LYS	734	1.491	60.104	29.739
502	CD	LYS	734	1.325	61.613	29.489
503	CE	LYS	734	-0.138	62.049	29.374
504	NZ	LYS	734	-0.392	63.445	29.911
505	HZ1	LYS	734	0.444	64.028	29.762
506	HZ2	LYS	734	-1.194	63.863	29.418
507	HZ3	LYS	734	-0.593	63.395	30.890
508	N	SER	735	-0.446	56.695	27.130
509	CA	SER	735	-1.555	55.887	26.617
510	HN	SER	735	0.211	57.099	26.494
511	C	SER	735	-1.320	54.381	26.706
512	O	SER	735	-2.236	53.585	26.468
513	CB	SER	735	-1.872	56.330	25.167
514	OG	SER	735	-0.870	55.921	24.229
515	HG	SER	735	-0.051	56.360	24.473
516	N	LEU	736	-0.098	53.982	27.036
517	CA	LEU	736	0.201	52.564	27.138
518	HN	LEU	736	0.618	54.658	27.214
519	C	LEU	736	-0.492	51.986	28.360
520	O	LEU	736	-0.279	52.425	29.492
521	CB	LEU	736	1.737	52.337	27.211
522	CG	LEU	736	2.577	52.603	25.932
523	CD1	LEU	736	4.063	52.733	26.294
524	CD2	LEU	736	2.398	51.510	24.866
525	N	PRO	737	-1.364	51.004	28.133
526	CA	PRO	737	-2.117	50.324	29.181
527	CD	PRO	737	-1.813	50.558	26.805
528	C	PRO	737	-1.207	49.971	30.340
529	O	PRO	737	-0.257	49.205	30.179
530	CB	PRO	737	-2.634	49.094	28.460
531	CG	PRO	737	-2.974	49.632	27.153
532	N	GLY	738	-1.488	50.541	31.504
533	CA	GLY	738	-0.686	50.263	32.676
534	HN	GLY	738	-2.263	51.169	31.573
535	C	GLY	738	0.524	51.152	32.913
536	O	GLY	738	1.221	50.970	33.900
537	N	PHE	739	0.796	52.120	32.039
538	CA	PHE	739	1.968	52.963	32.256
539	HN	PHE	739	0.206	52.267	31.245
540	C	PHE	739	1.713	54.100	33.242
541	O	PHE	739	2.584	54.419	34.053
542	CB	PHE	739	2.475	53.554	30.937
543	CG	PHE	739	3.713	54.395	31.096
544	CD1	PHE	739	4.959	53.797	31.287
545	CE1	PHE	739	6.098	54.575	31.517
546	CZ	PHE	739	5.992	55.961	31.555
547	CE2	PHE	739	4.751	56.569	31.359
548	CD2	PHE	739	3.623	55.785	31.127
549	N	ARG	740	0.528	54.705	33.164
550	CA	ARG	740	0.151	55.833	34.029

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551	HN	ARG	740	-0.132	54.378	32.488
552	C	ARG	740	0.051	55.468	35.498
553	O	ARG	740	0.347	56.277	36.381
554	CB	ARG	740	-1.196	56.436	33.600
555	CG	ARG	740	-1.600	57.692	34.347
556	CD	ARG	740	-2.959	58.220	33.899
557	NE	ARG	740	-3.349	59.432	34.619
558	CZ	ARG	740	-4.486	60.105	34.429
559	NH1	ARG	740	-5.500	59.734	33.612
560	1HH1	ARG	740	-6.319	60.308	33.542
561	2HH1	ARG	740	-5.429	58.896	33.081
562	NH2	ARG	740	-4.647	61.253	35.141
563	1HH2	ARG	740	-5.492	61.780	35.040
564	2HH2	ARG	740	-3.926	61.556	35.761
565	HE	ARG	740	-2.715	59.784	35.307
566	N	ASN	741	-0.380	54.242	35.752
567	CA	ASN	741	-0.544	53.777	37.110
568	HN	ASN	741	-0.595	53.628	34.993
569	C	ASN	741	0.765	53.516	37.822
570	O	ASN	741	0.778	53.044	38.950
571	CB	ASN	741	-1.436	52.542	37.106
572	CG	ASN	741	-2.805	52.837	36.517
573	OD1	ASN	741	-3.261	52.166	35.586
574	ND2	ASN	741	-3.556	53.863	37.133
575	1HD2	ASN	741	-4.490	54.048	36.802
576	2HD2	ASN	741	-3.174	54.391	37.903
577	N	LEU	742	1.882	53.801	37.176
578	CA	LEU	742	3.131	53.615	37.881
579	HN	LEU	742	1.864	54.134	36.233
580	C	LEU	742	3.372	54.966	38.511
581	O	LEU	742	2.731	55.960	38.163
582	CB	LEU	742	4.285	53.273	36.943
583	CG	LEU	742	4.343	51.909	36.258
584	CD1	LEU	742	4.962	52.123	34.901
585	CD2	LEU	742	5.151	50.896	37.058
586	N	HIS	743	4.309	55.000	39.441
587	CA	HIS	743	4.627	56.232	40.110
588	HN	HIS	743	4.799	54.162	39.683
589	C	HIS	743	5.054	57.283	39.094
590	O	HIS	743	5.888	57.008	38.239
591	CB	HIS	743	5.742	55.981	41.108
592	CG	HIS	743	5.813	57.008	42.187
593	ND1	HIS	743	6.381	58.249	42.000
594	CE1	HIS	743	6.253	58.959	43.105
595	NE2	HIS	743	5.621	58.221	44.003
596	HE2	HIS	743	5.383	58.518	44.960
597	CD2	HIS	743	5.333	56.999	43.455
598	N	ILE	744	4.482	58.476	39.192
599	CA	ILE	744	4.813	59.579	38.294
600	HN	ILE	744	3.799	58.625	39.907
601	C	ILE	744	6.313	59.875	38.306
602	O	ILE	744	6.792	60.726	37.559
603	CB	ILE	744	3.959	60.842	38.722
604	CG1	ILE	744	3.695	61.869	37.574
605	CG2	ILE	744	4.582	61.612	39.927

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606	CD1	ILE	744	2.243	61.944	37.059
607	N	ASP	745	7.044	59.181	39.173
608	CA	ASP	745	8.488	59.358	39.290
609	HN	ASP	745	6.590	58.516	39.764
610	C	ASP	745	9.214	58.319	38.448
611	O	ASP	745	10.326	58.563	37.974
612	CB	ASP	745	8.916	59.232	40.757
613	CG	ASP	745	9.276	60.572	41.382
614	OD1	ASP	745	8.646	61.590	41.021
615	OD2	ASP	745	10.184	60.599	42.245
616	HD2	ASP	745	10.305	61.486	42.548
617	N	ASP	746	8.597	57.155	38.283
618	CA	ASP	746	9.175	56.089	37.469
619	HN	ASP	746	7.714	57.004	38.728
620	C	ASP	746	8.833	56.439	36.039
621	O	ASP	746	9.643	56.265	35.127
622	CB	ASP	746	8.558	54.740	37.817
623	CG	ASP	746	8.720	54.394	39.271
624	OD1	ASP	746	9.723	54.839	39.871
625	OD2	ASP	746	7.853	53.670	39.809
626	HD2	ASP	746	8.076	53.533	40.717
627	N	GLN	747	7.603	56.923	35.872
628	CA	GLN	747	7.092	57.359	34.588
629	HN	GLN	747	7.005	56.988	36.671
630	C	GLN	747	8.132	58.302	34.013
631	O	GLN	747	8.317	58.385	32.802
632	CB	GLN	747	5.757	58.103	34.767
633	CG	GLN	747	4.525	57.205	34.669
634	CD	GLN	747	3.203	57.950	34.838
635	OE1	GLN	747	2.880	58.872	34.083
636	NE2	GLN	747	2.575	57.795	36.072
637	IHE2	GLN	747	1.680	58.234	36.220
638	2HE2	GLN	747	2.839	57.042	36.695
639	N	ILE	748	8.829	59.003	34.899
640	CA	ILE	748	9.852	59.943	34.473
641	HN	ILE	748	8.647	58.882	35.875
642	C	ILE	748	11.220	59.333	34.340
643	O	ILE	748	12.079	59.902	33.666
644	CB	ILE	748	9.852	61.182	35.458
645	CG1	ILE	748	8.996	62.397	34.977
646	CG2	ILE	748	11.288	61.698	35.781
647	CD1	ILE	748	9.230	63.724	35.728
648	N	THR	749	11.455	58.200	34.992
649	CA	THR	749	12.771	57.598	34.869
650	HN	THR	749	10.745	57.772	35.552
651	C	THR	749	12.803	56.821	33.566
652	O	THR	749	13.748	56.931	32.777
653	CB	THR	749	13.094	56.634	36.027
654	OG1	THR	749	12.430	56.896	37.254
655	HG1	THR	749	12.611	56.151	37.839
656	CG2	THR	749	14.573	56.755	36.400
657	N	LEU	750	11.745	56.053	33.341
658	CA	LEU	750	11.639	55.250	32.143
659	HN	LEU	750	11.005	56.030	34.013
660	C	LEU	750	11.834	56.098	30.863

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661	O	LEU	750	12.645	55.741	30.008
662	CB	LEU	750	10.300	54.486	32.171
663	CG	LEU	750	10.163	53.478	33.338
664	CD1	LEU	750	8.820	52.765	33.259
665	CD2	LEU	750	11.295	52.451	33.306
666	N	ILE	751	11.143	57.233	30.745
667	CA	ILE	751	11.298	58.090	29.570
668	HN	ILE	751	10.510	57.502	31.470
669	C	ILE	751	12.635	58.751	29.471
670	O	ILE	751	13.027	59.243	28.416
671	CB	ILE	751	10.118	59.145	29.580
672	CG1	ILE	751	8.725	58.569	29.167
673	CG2	ILE	751	10.412	60.390	28.686
674	CD1	ILE	751	7.530	59.534	29.306
675	N	GLN	752	13.337	58.801	30.584
676	CA	GLN	752	14.626	59.444	30.567
677	HN	GLN	752	12.981	58.399	31.428
678	C	GLN	752	15.720	58.460	30.267
679	O	GLN	752	16.740	58.801	29.672
680	CB	GLN	752	14.864	60.136	31.890
681	CG	GLN	752	14.349	61.550	31.885
682	CD	GLN	752	14.080	62.051	33.272
683	OE1	GLN	752	14.762	61.667	34.231
684	NE2	GLN	752	12.982	62.864	33.554
685	1HE2	GLN	752	12.838	63.166	34.506
686	2HE2	GLN	752	12.311	63.088	32.846
687	N	TYR	753	15.499	57.221	30.677
688	CA	TYR	753	16.473	56.184	30.422
689	HN	TYR	753	14.654	57.002	31.165
690	C	TYR	753	16.332	55.637	29.012
691	O	TYR	753	17.282	55.096	28.463
692	CB	TYR	753	16.270	55.032	31.377
693	CG	TYR	753	16.891	55.184	32.734
694	CD1	TYR	753	16.859	56.394	33.424
695	CE1	TYR	753	17.361	56.485	34.721
696	CZ	TYR	753	17.891	55.346	35.321
697	OH	TYR	753	18.389	55.465	36.601
698	HH	TYR	753	19.130	54.856	36.698
699	CE2	TYR	753	17.930	54.150	34.650
700	CD2	TYR	753	17.437	54.076	33.369
701	N	SER	754	15.157	55.784	28.406
702	CA	SER	754	14.983	55.203	27.088
703	HN	SER	754	14.412	56.282	28.849
704	C	SER	754	14.524	56.053	25.911
705	O	SER	754	14.159	55.506	24.878
706	CB	SER	754	14.067	53.978	27.206
707	OG	SER	754	12.749	54.286	27.635
708	HG	SER	754	12.366	53.459	27.955
709	N	TRP	755	14.556	57.371	26.019
710	CA	TRP	755	14.089	58.170	24.891
711	HN	TRP	755	14.891	57.809	26.853
712	C	TRP	755	14.860	57.907	23.575
713	O	TRP	755	14.270	57.970	22.492
714	CB	TRP	755	14.082	59.679	25.243
715	CG	TRP	755	15.425	60.318	25.318

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716	CD1	TRP	755	16.307	60.264	26.362
717	NE1	TRP	755	17.499	60.846	26.005
718	CE2	TRP	755	17.406	61.298	24.713
719	CD2	TRP	755	16.107	60.984	24.251
720	HE1	TRP	755	18.305	60.928	26.592
721	CE3	TRP	755	15.747	61.347	22.945
722	CZ3	TRP	755	16.687	61.997	22.145
723	CH2	TRP	755	17.976	62.289	22.635
724	CZ2	TRP	755	18.350	61.949	23.912
725	N	MET	756	16.154	57.583	23.653
726	CA	MET	756	16.939	57.351	22.436
727	HN	MET	756	16.590	57.497	24.549
728	C	MET	756	16.665	55.975	21.840
729	O	MET	756	16.599	55.804	20.620
730	CB	MET	756	18.437	57.489	22.727
731	CG	MET	756	19.322	57.374	21.487
732	SD	MET	756	19.295	58.819	20.443
733	CE	MET	756	20.458	59.745	21.299
734	N	SER	757	16.525	54.998	22.724
735	CA	SER	757	16.219	53.640	22.332
736	HN	SER	757	16.636	55.206	23.696
737	C	SER	757	14.879	53.727	21.599
738	O	SER	757	14.704	53.143	20.535
739	CB	SER	757	16.131	52.775	23.583
740	OG	SER	757	17.395	52.602	24.175
741	HG	SER	757	17.229	52.241	25.055
742	N	LEU	758	13.941	54.491	22.162
743	CA	LEU	758	12.628	54.685	21.544
744	HN	LEU	758	14.141	54.944	23.031
745	C	LEU	758	12.713	55.412	20.187
746	O	LEU	758	12.055	55.016	19.208
747	CB	LEU	758	11.729	55.508	22.468
748	CG	LEU	758	11.119	54.808	23.674
749	CD1	LEU	758	10.281	55.784	24.452
750	CD2	LEU	758	10.279	53.654	23.205
751	N	MET	759	13.511	56.479	20.156
752	CA	MET	759	13.702	57.297	18.966
753	HN	MET	759	14.001	56.731	20.990
754	C	MET	759	14.433	56.546	17.852
755	O	MET	759	14.021	56.589	16.690
756	CB	MET	759	14.447	58.591	19.331
757	CG	MET	759	13.553	59.646	19.984
758	SD	MET	759	14.425	61.220	20.263
759	CE	MET	759	13.139	62.315	21.053
760	N	VAL	760	15.514	55.854	18.209
761	CA	VAL	760	16.279	55.089	17.224
762	HN	VAL	760	15.807	55.857	19.165
763	C	VAL	760	15.451	53.923	16.702
764	O	VAL	760	15.347	53.742	15.490
765	CB	VAL	760	17.632	54.577	17.860
766	CG1	VAL	760	17.508	53.476	18.950
767	CG2	VAL	760	18.639	54.017	16.827
768	N	PHE	761	14.847	53.138	17.595
769	CA	PHE	761	14.062	52.008	17.125
770	HN	PHE	761	14.933	53.324	18.573

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771	C	PHE	761	13.040	52.442	16.091
772	O	PHE	761	12.930	51.819	15.041
773	CB	PHE	761	13.341	51.305	18.259
774	CG	PHE	761	12.974	49.889	17.946
775	CD1	PHE	761	13.965	48.983	17.586
776	CE1	PHE	761	13.653	47.672	17.293
777	CZ	PHE	761	12.321	47.252	17.340
778	CE2	PHE	761	11.312	48.151	17.694
779	CD2	PHE	761	11.644	49.464	17.986
780	N	GLY	762	12.287	53.501	16.375
781	CA	GLY	762	11.305	53.994	15.417
782	HN	GLY	762	12.396	53.964	17.254
783	C	GLY	762	11.969	54.319	14.068
784	O	GLY	762	11.510	53.828	13.038
785	N	LEU	763	13.028	55.129	14.052
786	CA	LEU	763	13.708	55.432	12.787
787	HN	LEU	763	13.359	55.533	14.905
788	C	LEU	763	14.084	54.093	12.138
789	O	LEU	763	13.863	53.883	10.944
790	CB	LEU	763	14.968	56.282	13.031
791	CG	LEU	763	16.092	56.607	12.014
792	CD1	LEU	763	15.854	57.869	11.161
793	CD2	LEU	763	17.329	56.845	12.863
794	N	GLY	764	14.643	53.181	12.926
795	CA	GLY	764	14.999	51.900	12.361
796	HN	GLY	764	14.813	53.377	13.892
797	C	GLY	764	13.834	51.459	11.509
798	O	GLY	764	13.961	51.256	10.308
799	N	TRP	765	12.676	51.353	12.134
800	CA	TRP	765	11.460	50.940	11.462
801	HN	TRP	765	12.637	51.565	13.110
802	C	TRP	765	11.085	51.734	10.187
803	O	TRP	765	10.868	51.159	9.134
804	CB	TRP	765	10.334	50.995	12.476
805	CG	TRP	765	9.056	50.606	11.930
806	CD1	TRP	765	8.037	51.435	11.565
807	NE1	TRP	765	6.972	50.695	11.112
808	CE2	TRP	765	7.299	49.365	11.173
809	CD2	TRP	765	8.609	49.276	11.699
810	HE1	TRP	765	6.100	51.066	10.791
811	CE3	TRP	765	9.194	48.009	11.852
812	CZ3	TRP	765	8.448	46.879	11.513
813	CH2	TRP	765	7.139	47.004	11.001
814	CZ2	TRP	765	6.547	48.234	10.834
815	N	ARG	766	10.993	53.047	10.288
816	CA	ARG	766	10.647	53.869	9.138
817	HN	ARG	766	11.164	53.485	11.171
818	C	ARG	766	11.567	53.630	7.941
819	O	ARG	766	11.138	53.702	6.787
820	CB	ARG	766	10.709	55.349	9.519
821	CG	ARG	766	9.605	55.799	10.434
822	CD	ARG	766	9.469	57.293	10.363
823	NE	ARG	766	10.615	57.981	10.950
824	CZ	ARG	766	10.942	57.921	12.243
825	NH1	ARG	766	10.223	57.241	13.179

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826	1HH1	ARG	766	10.522	57.249	14.133
827	2HH1	ARG	766	9.402	56.748	12.898
828	NH2	ARG	766	12.050	58.599	12.645
829	1HH2	ARG	766	12.330	58.592	13.604
830	2HH2	ARG	766	12.572	59.116	11.966
831	HE	ARG	766	11.190	58.532	10.346
832	N	SER	767	12.833	53.352	8.234
833	CA	SER	767	13.858	53.113	7.230
834	HN	SER	767	13.095	53.305	9.198
835	C	SER	767	13.671	51.814	6.491
836	O	SER	767	13.787	51.732	5.269
837	CB	SER	767	15.220	53.082	7.901
838	OG	SER	767	15.599	54.311	8.521
839	HG	SER	767	16.377	54.104	9.055
840	N	TYR	768	13.406	50.789	7.273
841	CA	TYR	768	13.218	49.465	6.764
842	HN	TYR	768	13.335	50.941	8.259
843	C	TYR	768	11.985	49.344	5.896
844	O	TYR	768	11.951	48.557	4.958
845	CB	TYR	768	13.133	48.529	7.960
846	CG	TYR	768	12.233	47.343	7.789
847	CD1	TYR	768	12.484	46.385	6.810
848	CE1	TYR	768	11.714	45.239	6.715
849	CZ	TYR	768	10.673	45.040	7.611
850	OH	TYR	768	9.912	43.894	7.529
851	HH	TYR	768	9.463	43.774	8.376
852	CE2	TYR	768	10.399	45.989	8.590
853	CD2	TYR	768	11.177	47.133	8.670
854	N	LYS	769	10.970	50.138	6.171
855	CA	LYS	769	9.756	49.993	5.397
856	HN	LYS	769	11.037	50.823	6.897
857	C	LYS	769	9.638	50.815	4.144
858	O	LYS	769	8.932	50.439	3.209
859	CB	LYS	769	8.566	50.268	6.357
860	CG	LYS	769	8.565	49.361	7.613
861	CD	LYS	769	7.176	48.937	8.100
862	CE	LYS	769	7.046	47.412	7.991
863	NZ	LYS	769	5.686	47.067	7.542
864	HZ2	LYS	769	5.346	47.752	6.857
865	HZ1	LYS	769	5.669	46.157	7.069
866	HZ3	LYS	769	5.070	47.045	8.330
867	N	HIS	770	10.348	51.932	4.147
868	CA	HIS	770	10.323	52.902	3.073
869	HN	HIS	770	10.934	52.116	4.936
870	C	HIS	770	11.406	52.732	2.021
871	O	HIS	770	11.350	53.354	0.962
872	CB	HIS	770	10.420	54.294	3.720
873	CG	HIS	770	9.805	55.363	2.866
874	ND1	HIS	770	9.981	56.736	3.026
875	CE1	HIS	770	9.222	57.185	2.008
876	NE2	HIS	770	8.584	56.268	1.231
877	CD2	HIS	770	8.969	55.080	1.795
878	HE2	HIS	770	7.968	56.421	0.419
879	N	VAL	771	12.404	51.906	2.311
880	CA	VAL	771	13.502	51.711	1.378

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881	HN	VAL	771	12.401	51.414	3.181
882	C	VAL	771	14.375	50.537	1.784
883	O	VAL	771	15.610	50.602	1.730
884	CB	VAL	771	14.356	53.036	1.270
885	CG1	VAL	771	14.529	53.853	2.580
886	CG2	VAL	771	15.790	52.816	0.733
887	N	SER	772	13.702	49.482	2.233
888	CA	SER	772	14.314	48.218	2.620
889	HN	SER	772	12.708	49.561	2.310
890	C	SER	772	15.612	48.239	3.458
891	O	SER	772	16.410	47.298	3.378
892	CB	SER	772	14.528	47.410	1.335
893	OG	SER	772	13.975	47.893	0.103
894	HG	SER	772	14.283	47.293	-0.588
895	N	GLY	773	15.798	49.283	4.266
896	CA	GLY	773	16.989	49.450	5.119
897	HN	GLY	773	15.092	49.990	4.295
898	C	GLY	773	18.206	49.933	4.318
899	O	GLY	773	19.350	49.548	4.604
900	N	GLN	774	17.949	50.786	3.330
901	CA	GLN	774	18.986	51.346	2.466
902	HN	GLN	774	17.000	51.058	3.171
903	C	GLN	774	19.341	52.784	2.844
904	O	GLN	774	20.516	53.158	2.902
905	CB	GLN	774	18.484	51.265	1.008
906	CG	GLN	774	18.381	49.831	0.391
907	CD	GLN	774	19.507	49.326	-0.520
908	OE1	GLN	774	19.482	48.199	-0.988
909	NE2	GLN	774	20.528	50.100	-0.787
910	2HE2	GLN	774	20.522	51.002	-0.309
911	1HE2	GLN	774	21.264	49.665	-1.347
912	N	MET	775	18.294	53.567	3.089
913	CA	MET	775	18.370	54.983	3.462
914	HN	MET	775	17.384	53.158	3.015
915	C	MET	775	17.939	55.180	4.938
916	O	MET	775	17.228	54.341	5.487
917	CB	MET	775	17.442	55.779	2.503
918	CG	MET	775	18.095	56.282	1.197
919	SD	MET	775	19.266	55.057	0.589
920	CE	MET	775	20.099	56.071	-0.639
921	N	LEU	776	18.401	56.252	5.592
922	CA	LEU	776	17.987	56.552	6.973
923	HN	LEU	776	19.044	56.864	5.132
924	C	LEU	776	16.867	57.558	6.762
925	O	LEU	776	17.090	58.616	6.182
926	CB	LEU	776	19.116	57.191	7.807
927	CG	LEU	776	20.065	56.240	8.555
928	CD1	LEU	776	20.964	57.020	9.506
929	CD2	LEU	776	19.243	55.216	9.333
930	N	TYR	777	15.670	57.231	7.238
931	CA	TYR	777	14.513	58.088	6.999
932	HN	TYR	777	15.561	56.388	7.766
933	C	TYR	777	13.906	58.809	8.186
934	O	TYR	777	12.846	58.426	8.682
935	CB	TYR	777	13.390	57.253	6.318

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936	CG	TYR	777	13.796	56.417	5.100
937	CD1	TYR	777	13.972	57.016	3.849
938	CD2	TYR	777	14.003	55.041	5.240
939	CE1	TYR	777	14.357	56.247	2.753
940	CE2	TYR	777	14.387	54.274	4.144
941	CZ	TYR	777	14.563	54.878	2.901
942	OH	TYR	777	14.943	54.128	1.825
943	HH	TYR	777	15.041	53.217	2.109
944	N	PHE	778	14.541	59.887	8.604
945	CA	PHE	778	14.068	60.646	9.741
946	HN	PHE	778	15.367	60.186	8.125
947	C	PHE	778	12.603	61.090	9.692
948	O	PHE	778	11.859	60.829	10.642
949	CB	PHE	778	15.020	61.807	9.972
950	CG	PHE	778	16.386	61.318	10.325
951	CD1	PHE	778	17.224	60.778	9.351
952	CE1	PHE	778	18.446	60.198	9.699
953	CZ	PHE	778	18.886	60.261	11.009
954	CE2	PHE	778	18.061	60.811	11.987
955	CD2	PHE	778	16.845	61.390	11.630
956	N	ALA	779	12.191	61.735	8.605
957	CA	ALA	779	10.803	62.195	8.413
958	HN	ALA	779	12.856	61.919	7.881
959	C	ALA	779	10.591	62.160	6.899
960	O	ALA	779	11.186	62.970	6.216
961	CB	ALA	779	10.644	63.625	8.933
962	N	PRO	780	9.756	61.236	6.359
963	CA	PRO	780	9.579	61.215	4.895
964	CD	PRO	780	8.903	60.205	6.984
965	C	PRO	780	9.892	62.462	4.031
966	O	PRO	780	10.012	62.338	2.812
967	CB	PRO	780	8.151	60.692	4.748
968	CG	PRO	780	8.154	59.579	5.772
969	N	ASP	781	10.023	63.635	4.660
970	CA	ASP	781	10.403	64.883	3.987
971	HN	ASP	781	9.853	63.663	5.645
972	C	ASP	781	11.908	65.110	4.248
973	O	ASP	781	12.416	66.219	4.071
974	CB	ASP	781	9.547	66.079	4.513
975	CG	ASP	781	10.321	67.074	5.442
976	OD1	ASP	781	11.387	66.743	6.007
977	OD2	ASP	781	9.831	68.214	5.632
978	HD2	ASP	781	10.395	68.707	6.208
979	N	LEU	782	12.622	64.067	4.686
980	CA	LEU	782	14.066	64.183	4.963
981	HN	LEU	782	12.166	63.188	4.829
982	C	LEU	782	14.766	62.853	5.221
983	O	LEU	782	14.845	62.374	6.362
984	CB	LEU	782	14.356	65.126	6.149
985	CG	LEU	782	15.833	65.518	6.400
986	CD1	LEU	782	15.922	66.482	7.567
987	CD2	LEU	782	16.696	64.304	6.705
988	N	ILE	783	15.304	62.307	4.134
989	CA	ILE	783	16.033	61.049	4.107
990	HN	ILE	783	15.199	62.799	3.270

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991	C	ILE	783	17.515	61.321	3.918
992	O	ILE	783	17.910	62.236	3.195
993	CB	ILE	783	15.594	60.191	2.921
994	CG2	ILE	783	16.348	58.883	2.912
995	CG1	ILE	783	14.084	59.984	2.973
996	CD1	ILE	783	13.580	58.911	2.035
997	N	LEU	784	18.352	60.533	4.567
998	CA	LEU	784	19.752	60.743	4.372
999	HN	LEU	784	18.017	59.814	5.176
1000	C	LEU	784	20.207	59.721	3.381
1001	O	LEU	784	20.504	58.575	3.718
1002	CB	LEU	784	20.567	60.640	5.692
1003	CG	LEU	784	20.745	61.925	6.544
1004	CD1	LEU	784	21.240	61.561	7.951
1005	CD2	LEU	784	21.709	62.936	5.901
1006	N	ASN	785	20.172	60.171	2.136
1007	CA	ASN	785	20.583	59.440	0.952
1008	HN	ASN	785	19.831	61.101	1.999
1009	C	ASN	785	22.105	59.406	0.993
1010	O	ASN	785	22.741	59.804	1.982
1011	CB	ASN	785	20.158	60.228	-0.266
1012	CG	ASN	785	20.463	61.686	-0.088
1013	OD1	ASN	785	21.246	62.041	0.802
1014	ND2	ASN	785	19.835	62.588	-0.969
1015	1HD2	ASN	785	20.070	63.569	-0.935
1016	2HD2	ASN	785	19.233	62.251	-1.704
1017	N	GLU	786	22.663	58.979	-0.126
1018	CA	GLU	786	24.082	58.822	-0.276
1019	HN	GLU	786	22.072	58.756	-0.901
1020	C	GLU	786	24.617	60.138	-0.412
1021	O	GLU	786	25.341	60.550	0.437
1022	CB	GLU	786	24.391	58.080	-1.511
1023	CG	GLU	786	25.667	57.375	-1.441
1024	CD	GLU	786	26.031	56.969	-2.820
1025	OE1	GLU	786	25.501	55.940	-3.297
1026	OE2	GLU	786	26.811	57.715	-3.446
1027	HE2	GLU	786	26.969	57.356	-4.306
1028	N	GLN	787	24.351	60.774	-1.523
1029	CA	GLN	787	24.794	62.102	-1.541
1030	HN	GLN	787	23.873	60.349	-2.292
1031	C	GLN	787	25.042	62.437	-0.030
1032	O	GLN	787	26.119	62.188	0.452
1033	CB	GLN	787	23.667	62.852	-2.085
1034	CG	GLN	787	24.038	64.078	-2.608
1035	CD	GLN	787	22.876	64.912	-2.433
1036	OE1	GLN	787	21.774	64.528	-2.827
1037	NE2	GLN	787	23.064	66.159	-1.785
1038	1HE2	GLN	787	22.280	66.783	-1.655
1039	2HE2	GLN	787	23.984	66.437	-1.479
1040	N	ARG	788	24.048	62.861	0.759
1041	CA	ARG	788	24.284	63.236	2.187
1042	HN	ARG	788	23.124	62.930	0.385
1043	C	ARG	788	25.212	62.467	3.112
1044	O	ARG	788	26.035	63.039	3.822
1045	CB	ARG	788	22.962	63.385	2.896

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1046	CG	ARG	788	22.235	64.527	2.333
1047	CD	ARG	788	20.817	64.471	2.706
1048	NE	ARG	788	20.155	65.689	2.277
1049	CZ	ARG	788	18.843	65.836	2.288
1050	NH1	ARG	788	17.944	64.906	2.689
1051	1HH1	ARG	788	16.968	65.106	2.663
1052	2HH1	ARG	788	18.268	64.016	3.011
1053	NH2	ARG	788	18.393	67.046	1.851
1054	1HH2	ARG	788	17.416	67.245	1.824
1055	2HH2	ARG	788	19.071	67.726	1.561
1056	HE	ARG	788	20.719	66.452	1.960
1057	N	MET	789	25.022	61.164	3.130
1058	CA	MET	789	25.809	60.250	3.920
1059	HN	MET	789	24.290	60.787	2.563
1060	C	MET	789	27.284	60.373	3.637
1061	O	MET	789	28.101	59.697	4.243
1062	CB	MET	789	25.429	58.865	3.514
1063	CG	MET	789	24.167	58.419	4.097
1064	SD	MET	789	23.912	56.709	3.659
1065	CE	MET	789	22.418	56.454	4.443
1066	N	LYS	790	27.641	61.215	2.696
1067	CA	LYS	790	29.031	61.282	2.344
1068	HN	LYS	790	26.965	61.793	2.238
1069	C	LYS	790	29.746	62.384	3.101
1070	O	LYS	790	30.975	62.481	3.039
1071	CB	LYS	790	29.122	61.512	0.810
1072	CG	LYS	790	27.919	62.298	0.233
1073	CD	LYS	790	27.941	62.487	-1.286
1074	CE	LYS	790	26.663	63.214	-1.725
1075	NZ	LYS	790	26.758	63.551	-3.157
1076	HZ2	LYS	790	27.235	62.803	-3.674
1077	HZ1	LYS	790	25.829	63.643	-3.580
1078	HZ3	LYS	790	27.261	64.408	-3.265
1079	N	GLU	791	28.943	63.122	3.884
1080	CA	GLU	791	29.321	64.309	4.668
1081	HN	GLU	791	27.987	62.835	3.941
1082	C	GLU	791	30.190	64.269	5.882
1083	O	GLU	791	29.802	63.817	6.953
1084	CB	GLU	791	28.014	65.107	4.935
1085	CG	GLU	791	27.277	65.712	3.694
1086	CD	GLU	791	27.943	66.869	2.946
1087	OE1	GLU	791	28.629	67.715	3.503
1088	OE2	GLU	791	27.700	66.866	1.606
1089	HE2	GLU	791	28.137	67.602	1.205
1090	N	SER	792	31.290	64.992	5.774
1091	HN	SER	792	31.460	65.527	4.911
1092	CA	SER	792	32.264	65.049	6.850
1093	C	SER	792	32.067	64.179	8.078
1094	O	SER	792	32.972	63.485	8.496
1095	CB	SER	792	32.290	66.554	7.217
1096	OG	SER	792	32.013	67.404	6.098
1097	HG	SER	792	32.714	67.269	5.455
1098	N	SER	793	30.907	64.132	8.672
1099	CA	SER	793	30.965	63.399	9.897
1100	HN	SER	793	30.077	64.558	8.313

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1101	C	SER	793	29.791	62.534	10.105
1102	O	SER	793	29.540	62.065	11.206
1103	CB	SER	793	31.071	64.489	10.994
1104	OG	SER	793	32.304	64.430	11.719
1105	HG	SER	793	32.330	63.584	12.174
1106	N	PHE	794	29.108	62.259	9.021
1107	CA	PHE	794	27.866	61.582	9.147
1108	HN	PHE	794	29.455	62.522	8.121
1109	C	PHE	794	27.801	60.103	9.326
1110	O	PHE	794	27.198	59.595	10.283
1111	CB	PHE	794	26.966	61.982	7.939
1112	CG	PHE	794	26.406	63.413	7.948
1113	CD1	PHE	794	26.710	64.269	9.013
1114	CE1	PHE	794	26.147	65.538	9.076
1115	CZ	PHE	794	25.289	65.968	8.067
1116	CE2	PHE	794	24.990	65.126	6.997
1117	CD2	PHE	794	25.545	63.850	6.938
1118	N	TYR	795	28.424	59.411	8.394
1119	CA	TYR	795	28.382	57.988	8.407
1120	HN	TYR	795	28.928	59.887	7.673
1121	C	TYR	795	28.762	57.515	9.775
1122	O	TYR	795	28.033	56.784	10.449
1123	CB	TYR	795	29.348	57.438	7.376
1124	CG	TYR	795	29.176	55.974	7.269
1125	CD1	TYR	795	28.002	55.450	6.752
1126	CE1	TYR	795	27.745	54.108	6.812
1127	CZ	TYR	795	28.671	53.268	7.389
1128	OH	TYR	795	28.414	51.916	7.449
1129	HH	TYR	795	29.242	51.461	7.639
1130	CE2	TYR	795	29.855	53.763	7.897
1131	CD2	TYR	795	30.101	55.111	7.832
1132	N	SER	796	29.891	58.001	10.221
1133	CA	SER	796	30.342	57.544	11.482
1134	HN	SER	796	30.414	58.669	9.692
1135	C	SER	796	29.351	57.385	12.601
1136	O	SER	796	29.510	56.535	13.475
1137	CB	SER	796	31.546	58.421	11.908
1138	OG	SER	796	32.608	57.662	12.496
1139	HG	SER	796	32.265	57.264	13.300
1140	N	LEU	797	28.310	58.183	12.555
1141	CA	LEU	797	27.317	58.140	13.581
1142	HN	LEU	797	28.212	58.827	11.796
1143	C	LEU	797	26.033	57.625	13.033
1144	O	LEU	797	25.110	57.369	13.780
1145	CB	LEU	797	27.158	59.601	14.089
1146	CG	LEU	797	28.428	60.347	14.580
1147	CD1	LEU	797	28.597	60.160	16.094
1148	CD2	LEU	797	29.704	59.888	13.856
1149	N	CYS	798	25.928	57.473	11.730
1150	CA	CYS	798	24.626	57.048	11.241
1151	HN	CYS	798	26.698	57.640	11.114
1152	C	CYS	798	24.672	55.630	11.032
1153	O	CYS	798	23.734	54.964	10.598
1154	CB	CYS	798	24.304	57.699	9.924
1155	SG	CYS	798	25.429	57.249	8.557

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1156	HG	CYS	798	25.052	57.880	7.443
1157	N	LEU	799	25.779	55.124	11.438
1158	CA	LEU	799	25.912	53.807	11.104
1159	HN	LEU	799	26.470	55.639	11.944
1160	C	LEU	799	25.261	52.926	12.098
1161	O	LEU	799	24.784	51.861	11.743
1162	CB	LEU	799	27.437	53.512	11.014
1163	CG	LEU	799	27.888	52.198	10.320
1164	CD1	LEU	799	29.402	52.227	10.070
1165	CD2	LEU	799	27.519	50.943	11.127
1166	N	THR	800	25.210	53.364	13.345
1167	CA	THR	800	24.614	52.485	14.303
1168	HN	THR	800	25.569	54.261	13.604
1169	C	THR	800	23.134	52.463	14.182
1170	O	THR	800	22.489	51.556	14.682
1171	CB	THR	800	25.044	52.867	15.760
1172	OG1	THR	800	26.408	52.530	15.980
1173	HG1	THR	800	26.624	52.853	16.860
1174	CG2	THR	800	24.282	52.165	16.905
1175	N	MET	801	22.602	53.452	13.488
1176	CA	MET	801	21.170	53.504	13.266
1177	HN	MET	801	23.189	54.169	13.114
1178	C	MET	801	20.868	52.600	12.120
1179	O	MET	801	19.942	51.793	12.150
1180	CB	MET	801	20.762	54.886	12.872
1181	CG	MET	801	20.691	55.778	14.039
1182	SD	MET	801	20.060	57.362	13.567
1183	CE	MET	801	21.271	57.817	12.406
1184	N	TRP	802	21.643	52.808	11.071
1185	CA	TRP	802	21.545	52.016	9.879
1186	HN	TRP	802	22.321	53.542	11.110
1187	C	TRP	802	21.468	50.589	10.305
1188	O	TRP	802	20.836	49.738	9.690
1189	CB	TRP	802	22.844	52.252	9.060
1190	CG	TRP	802	22.891	51.531	7.709
1191	CD1	TRP	802	22.891	51.531	7.709
1192	NE1	TRP	802	23.488	50.276	7.467
1193	CE2	TRP	802	23.432	49.930	6.103
1194	CD2	TRP	802	22.790	51.007	5.513
1195	HE1	TRP	802	22.457	51.986	6.482
1196	CE3	TRP	802	23.821	49.099	5.643
1197	CZ3	TRP	802	21.816	53.192	6.099
1198	CH2	TRP	802	21.507	53.379	4.752
1199	CZ2	TRP	802	21.828	52.408	3.793
1200	N	GLN	803	22.472	51.222	4.154
1201	CA	GLN	803	22.153	50.339	11.396
1202	HN	GLN	803	22.243	49.017	11.904
1203	C	GLN	803	22.616	51.086	11.873
1204	O	GLN	803	20.950	48.353	12.340
1205	CB	GLN	803	20.775	47.145	12.174
1206	CG	GLN	803	23.270	49.040	13.058
1207	CD	GLN	803	23.347	47.750	13.940
1208	OE1	GLN	803	23.993	46.486	13.360
1209	NE2	GLN	803	23.982	45.432	13.976
1210	2HE2	GLN	803	24.591	46.532	12.197
				24.626	47.457	11.766

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1211	IHE2	GLN	803	25.051	45.665	11.913
1212	N	ILE	804	20.050	49.131	12.906
1213	CA	ILE	804	18.817	48.561	13.415
1214	HN	ILE	804	20.217	50.114	12.985
1215	C	ILE	804	17.808	48.322	12.301
1216	O	ILE	804	17.107	47.307	12.280
1217	CB	ILE	804	18.233	49.500	14.547
1218	CG1	ILE	804	19.231	50.578	15.080
1219	CG2	ILE	804	17.683	48.703	15.770
1220	CD1	ILE	804	18.615	51.703	15.936
1221	N	PRO	805	17.761	49.278	11.384
1222	CA	PRO	805	16.882	49.259	10.220
1223	C	PRO	805	17.249	48.056	9.390
1224	O	PRO	805	16.449	47.474	8.650
1225	CB	PRO	805	17.108	50.588	9.484
1226	CG	PRO	805	18.553	50.963	9.848
1227	CD	PRO	805	18.675	50.520	11.308
1228	N	GLN	806	18.511	47.706	9.525
1229	CA	GLN	806	19.063	46.614	8.791
1230	HN	GLN	806	19.095	48.217	10.156
1231	C	GLN	806	18.670	45.295	9.410
1232	O	GLN	806	18.528	44.284	8.737
1233	CB	GLN	806	20.598	46.786	8.783
1234	CG	GLN	806	21.441	45.470	8.858
1235	CD	GLN	806	22.971	45.564	8.916
1236	OE1	GLN	806	23.661	44.563	9.015
1237	NE2	GLN	806	23.555	46.735	8.884
1238	2HE2	GLN	806	22.920	47.534	8.870
1239	1HE2	GLN	806	24.571	46.713	8.992
1240	N	GLU	807	18.482	45.308	10.714
1241	CA	GLU	807	18.132	44.091	11.393
1242	HN	GLU	807	18.583	46.160	11.228
1243	C	GLU	807	16.669	43.824	11.239
1244	O	GLU	807	16.231	42.679	11.130
1245	CB	GLU	807	18.518	44.229	12.845
1246	CG	GLU	807	19.997	44.150	12.996
1247	CD	GLU	807	20.469	42.740	12.723
1248	OE1	GLU	807	20.203	41.865	13.569
1249	OE2	GLU	807	21.082	42.493	11.663
1250	HE2	GLU	807	21.309	41.576	11.637
1251	N	PHE	808	15.910	44.900	11.228
1252	CA	PHE	808	14.478	44.796	11.066
1253	HN	PHE	808	16.330	45.802	11.332
1254	C	PHE	808	14.232	44.138	9.744
1255	O	PHE	808	13.408	43.246	9.581
1256	CB	PHE	808	13.861	46.228	11.038
1257	CG	PHE	808	13.638	46.903	12.400
1258	CD1	PHE	808	13.232	48.242	12.450
1259	CE1	PHE	808	13.103	48.891	13.673
1260	CZ	PHE	808	13.363	48.202	14.855
1261	CE2	PHE	808	13.757	46.866	14.814
1262	CD2	PHE	808	13.897	46.218	13.589
1263	N	VAL	809	14.977	44.617	8.782
1264	CA	VAL	809	14.838	44.102	7.476
1265	HN	VAL	809	15.639	45.342	8.971

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1266	C	VAL	809	15.236	42.654	7.417
1267	O	VAL	809	14.511	41.796	6.912
1268	CB	VAL	809	15.760	44.976	6.536
1269	CG1	VAL	809	15.758	44.603	5.028
1270	CG2	VAL	809	15.445	46.491	6.582
1271	N	LYS	810	16.426	42.387	7.907
1272	CA	LYS	810	16.928	41.042	7.870
1273	HN	LYS	810	16.981	43.119	8.304
1274	C	LYS	810	16.024	40.070	8.594
1275	O	LYS	810	15.810	38.937	8.166
1276	CB	LYS	810	18.353	41.041	8.489
1277	CG	LYS	810	18.830	39.637	8.937
1278	CD	LYS	810	20.248	39.591	9.511
1279	CE	LYS	810	20.176	39.645	11.043
1280	NZ	LYS	810	19.606	38.385	11.551
1281	HZ2	LYS	810	19.931	37.588	10.990
1282	HZ1	LYS	810	19.911	38.199	12.512
1283	HZ3	LYS	810	18.608	38.433	11.520
1284	N	LEU	811	15.495	40.520	9.712
1285	CA	LEU	811	14.655	39.668	10.510
1286	HN	LEU	811	15.678	41.458	10.007
1287	C	LEU	811	13.234	39.665	10.035
1288	O	LEU	811	12.397	38.918	10.547
1289	CB	LEU	811	14.713	40.140	11.936
1290	CG	LEU	811	15.052	39.039	12.925
1291	CD1	LEU	811	16.041	38.065	12.339
1292	CD2	LEU	811	15.613	39.703	14.158
1293	N	GLN	812	12.952	40.532	9.071
1294	CA	GLN	812	11.615	40.583	8.549
1295	HN	GLN	812	13.660	41.140	8.713
1296	C	GLN	812	10.696	40.731	9.721
1297	O	GLN	812	9.911	39.842	10.019
1298	CB	GLN	812	11.347	39.285	7.826
1299	CG	GLN	812	12.088	39.230	6.534
1300	CD	GLN	812	11.426	40.137	5.538
1301	OE1	GLN	812	12.016	41.104	5.053
1302	NE2	GLN	812	10.143	39.757	5.076
1303	1HE2	GLN	812	9.717	40.296	4.336
1304	2HE2	GLN	812	9.714	38.902	5.392
1305	N	VAL	813	10.802	41.849	10.410
1306	CA	VAL	813	9.957	42.060	11.554
1307	HN	VAL	813	11.466	42.546	10.139
1308	C	VAL	813	8.637	42.654	11.111
1309	O	VAL	813	8.601	43.514	10.245
1310	CB	VAL	813	10.678	42.954	12.576
1311	CG1	VAL	813	9.686	43.569	13.534
1312	CG2	VAL	813	11.707	42.109	13.330
1313	N	SER	814	7.550	42.174	11.707
1314	CA	SER	814	6.206	42.646	11.374
1315	HN	SER	814	7.654	41.466	12.405
1316	C	SER	814	5.740	43.761	12.307
1317	O	SER	814	6.142	43.810	13.468
1318	CB	SER	814	5.222	41.499	11.479
1319	OG	SER	814	4.854	41.159	12.814
1320	HG	SER	814	4.170	40.479	12.754

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1321	N	GLN	815	4.866	44.635	11.811
1322	CA	GLN	815	4.351	45.754	12.613
1323	HN	GLN	815	4.552	44.527	10.867
1324	C	GLN	815	3.904	45.330	13.998
1325	O	GLN	815	4.118	46.035	14.988
1326	CB	GLN	815	3.195	46.426	11.840
1327	CG	GLN	815	2.824	47.881	12.278
1328	CD	GLN	815	3.920	48.953	12.315
1329	OE1	GLN	815	3.652	50.122	12.543
1330	NE2	GLN	815	5.164	48.624	12.073
1331	2HE2	GLN	815	5.311	47.646	11.821
1332	1HE2	GLN	815	5.821	49.407	12.053
1333	N	GLU	816	3.249	44.187	14.073
1334	CA	GLU	816	2.791	43.772	15.369
1335	HN	GLU	816	3.079	43.631	13.259
1336	C	GLU	816	3.939	43.440	16.298
1337	O	GLU	816	3.918	43.859	17.456
1338	CB	GLU	816	1.775	42.645	15.241
1339	CG	GLU	816	0.366	43.221	15.199
1340	CD	GLU	816	-0.716	42.166	15.204
1341	OE1	GLU	816	-0.619	41.208	16.010
1342	OE2	GLU	816	-1.673	42.306	14.407
1343	HE2	GLU	816	-2.276	41.586	14.509
1344	N	GLU	817	4.954	42.726	15.821
1345	CA	GLU	817	6.095	42.447	16.690
1346	HN	GLU	817	4.937	42.386	14.881
1347	C	GLU	817	6.767	43.775	17.046
1348	O	GLU	817	7.106	44.024	18.195
1349	CB	GLU	817	7.107	41.550	15.999
1350	CG	GLU	817	6.523	40.254	15.554
1351	CD	GLU	817	7.381	39.567	14.525
1352	OE1	GLU	817	7.888	40.268	13.614
1353	OE2	GLU	817	7.534	38.332	14.621
1354	HE2	GLU	817	8.090	38.028	13.919
1355	N	PHE	818	6.961	44.631	16.052
1356	CA	PHE	818	7.599	45.926	16.270
1357	HN	PHE	818	6.663	44.383	15.130
1358	C	PHE	818	6.930	46.789	17.341
1359	O	PHE	818	7.599	47.422	18.157
1360	CB	PHE	818	7.619	46.716	14.927
1361	CG	PHE	818	7.823	48.236	15.031
1362	CD1	PHE	818	9.110	48.750	15.221
1363	CE1	PHE	818	9.326	50.123	15.217
1364	CZ	PHE	818	8.258	50.993	15.006
1365	CE2	PHE	818	6.975	50.488	14.804
1366	CD2	PHE	818	6.756	49.113	14.818
1367	N	LEU	819	5.608	46.853	17.289
1368	CA	LEU	819	4.847	47.635	18.238
1369	HN	LEU	819	5.123	46.347	16.575
1370	C	LEU	819	5.158	47.193	19.666
1371	O	LEU	819	5.472	48.013	20.534
1372	CB	LEU	819	3.348	47.483	17.961
1373	CG	LEU	819	2.776	48.377	16.869
1374	CD1	LEU	819	1.284	48.208	16.796
1375	CD2	LEU	819	3.116	49.813	17.180

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1376	N	CYS	820	5.049	45.886	19.882
1377	CA	CYS	820	5.315	45.273	21.168
1378	HN	CYS	820	4.771	45.298	19.122
1379	C	CYS	820	6.753	45.478	21.587
1380	O	CYS	820	7.049	45.668	22.759
1381	CB	CYS	820	5.047	43.781	21.103
1382	SG	CYS	820	3.280	43.364	20.905
1383	HG	CYS	820	3.138	42.038	20.857
1384	N	MET	821	7.657	45.430	20.633
1385	CA	MET	821	9.054	45.604	20.957
1386	HN	MET	821	7.378	45.273	19.686
1387	C	MET	821	9.407	47.017	21.406
1388	O	MET	821	10.286	47.205	22.252
1389	CB	MET	821	9.920	45.227	19.760
1390	CG	MET	821	10.038	43.744	19.538
1391	SD	MET	821	11.149	43.450	18.194
1392	CE	MET	821	10.046	43.457	16.968
1393	N	LYS	822	8.738	48.013	20.833
1394	CA	LYS	822	9.021	49.393	21.192
1395	HN	LYS	822	8.035	47.811	20.150
1396	C	LYS	822	8.476	49.690	22.582
1397	O	LYS	822	9.008	50.541	23.304
1398	CB	LYS	822	8.393	50.324	20.170
1399	CG	LYS	822	8.973	51.714	20.152
1400	CD	LYS	822	8.431	52.481	18.948
1401	CE	LYS	822	6.976	52.947	19.146
1402	NZ	LYS	822	5.879	51.911	19.313
1403	HZ1	LYS	822	4.968	52.385	19.393
1404	HZ2	LYS	822	5.869	51.286	18.495
1405	HZ3	LYS	822	6.049	51.374	20.139
1406	N	VAL	823	7.405	48.990	22.947
1407	CA	VAL	823	6.794	49.152	24.249
1408	HN	VAL	823	7.012	48.333	22.304
1409	C	VAL	823	7.792	48.552	25.214
1410	O	VAL	823	8.098	49.138	26.238
1411	CB	VAL	823	5.416	48.382	24.314
1412	CG1	VAL	823	4.716	48.337	25.701
1413	CG2	VAL	823	4.347	48.924	23.335
1414	N	LEU	824	8.316	47.381	24.860
1415	CA	LEU	824	9.318	46.724	25.680
1416	HN	LEU	824	8.014	46.945	24.013
1417	C	LEU	824	10.542	47.619	25.856
1418	O	LEU	824	11.126	47.645	26.920
1419	CB	LEU	824	9.732	45.399	25.057
1420	CG	LEU	824	9.203	44.140	25.744
1421	CD1	LEU	824	8.142	44.484	26.747
1422	CD2	LEU	824	8.656	43.185	24.714
1423	N	LEU	825	10.939	48.369	24.839
1424	CA	LEU	825	12.107	49.226	25.037
1425	HN	LEU	825	10.456	48.350	23.963
1426	C	LEU	825	11.882	50.322	26.062
1427	O	LEU	825	12.837	50.825	26.638
1428	CB	LEU	825	12.541	49.892	23.740
1429	CG	LEU	825	13.182	49.049	22.650
1430	CD1	LEU	825	13.307	49.968	21.459

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1431	CD2	LEU	825	14.549	48.490	23.053
1432	N	LEU	826	10.630	50.712	26.265
1433	CA	LEU	826	10.312	51.764	27.230
1434	HN	LEU	826	9.890	50.278	25.750
1435	C	LEU	826	10.574	51.184	28.611
1436	O	LEU	826	10.954	51.899	29.541
1437	CB	LEU	826	8.840	52.169	27.109
1438	CG	LEU	826	8.322	53.116	28.189
1439	CD1	LEU	826	9.120	54.420	28.142
1440	CD2	LEU	826	6.831	53.361	27.988
1441	N	LEU	827	10.382	49.872	28.710
1442	CA	LEU	827	10.577	49.134	29.944
1443	HN	LEU	827	10.089	49.370	27.896
1444	C	LEU	827	11.923	48.441	29.920
1445	O	LEU	827	12.131	47.479	30.657
1446	CB	LEU	827	9.495	48.072	30.065
1447	CG	LEU	827	8.104	48.624	29.807
1448	CD1	LEU	827	7.060	47.528	29.964
1449	CD2	LEU	827	7.865	49.767	30.773
1450	N	ASN	828	12.837	48.936	29.093
1451	CA	ASN	828	14.140	48.299	28.921
1452	HN	ASN	828	12.627	49.766	28.575
1453	C	ASN	828	15.279	48.552	29.904
1454	O	ASN	828	16.359	47.972	29.754
1455	CB	ASN	828	14.611	48.542	27.457
1456	CG	ASN	828	15.909	47.853	27.023
1457	OD1	ASN	828	16.588	48.268	26.095
1458	ND2	ASN	828	16.289	46.773	27.651
1459	1HD2	ASN	828	17.076	46.309	27.188
1460	2HD2	ASN	828	15.655	46.401	28.358
1461	N	THR	829	15.084	49.428	30.877
1462	CA	THR	829	16.135	49.624	31.870
1463	HN	THR	829	14.231	49.947	30.930
1464	C	THR	829	15.597	50.417	33.047
1465	O	THR	829	14.769	51.313	32.899
1466	CB	THR	829	17.426	50.297	31.293
1467	OG1	THR	829	17.180	51.662	30.983
1468	HG1	THR	829	18.024	52.029	30.704
1469	CG2	THR	829	17.984	49.697	29.985
1470	N	ILE	830	16.033	50.023	34.233
1471	CA	ILE	830	15.585	50.666	35.447
1472	HN	ILE	830	16.684	49.267	34.291
1473	C	ILE	830	16.791	51.117	36.256
1474	O	ILE	830	17.930	50.741	35.961
1475	CB	ILE	830	14.665	49.670	36.265
1476	CG1	ILE	830	13.280	49.373	35.607
1477	CG2	ILE	830	14.414	50.145	37.730
1478	CD1	ILE	830	12.498	48.179	36.193
1479	N	PRO	831	16.563	51.958	37.275
1480	CA	PRO	831	17.668	52.431	38.099
1481	CD	PRO	831	15.277	52.419	37.819
1482	C	PRO	831	18.186	51.221	38.868
1483	O	PRO	831	17.402	50.334	39.217
1484	CB	PRO	831	16.993	53.465	38.994
1485	CG	PRO	831	15.648	52.866	39.206

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1486	N	LEU	832	19.494	51.150	39.095
1487	CA	LEU	832	20.052	50.018	39.834
1488	HN	LEU	832	20.098	51.873	38.760
1489	C	LEU	832	19.707	50.210	41.288
1490	O	LEU	832	20.462	50.805	42.041
1491	CB	LEU	832	21.592	49.932	39.634
1492	CG	LEU	832	22.428	49.192	40.713
1493	CD1	LEU	832	21.838	47.800	40.976
1494	CD2	LEU	832	23.911	49.063	40.329
1495	N	GLU	833	18.554	49.692	41.671
1496	CA	GLU	833	18.050	49.804	43.023
1497	HN	GLU	833	18.004	49.201	40.995
1498	C	GLU	833	16.579	49.552	42.796
1499	O	GLU	833	15.893	48.957	43.627
1500	CB	GLU	833	18.296	51.227	43.599
1501	CG	GLU	833	19.635	51.466	44.371
1502	CD	GLU	833	20.266	50.286	45.114
1503	OE1	GLU	833	21.328	50.371	45.718
1504	OE2	GLU	833	19.537	49.139	45.040
1505	HE2	GLU	833	19.980	48.453	45.517
1506	N	GLY	834	16.109	50.000	41.634
1507	CA	GLY	834	14.720	49.791	41.279
1508	HN	GLY	834	16.717	50.483	41.004
1509	C	GLY	834	13.826	50.996	41.429
1510	O	GLY	834	14.203	52.016	42.013
1511	N	LEU	835	12.610	50.858	40.909
1512	CA	LEU	835	11.630	51.928	40.943
1513	HN	LEU	835	12.364	49.989	40.480
1514	C	LEU	835	10.728	51.875	42.168
1515	O	LEU	835	10.668	50.869	42.873
1516	CB	LEU	835	10.747	51.874	39.691
1517	CG	LEU	835	11.282	51.133	38.465
1518	CD1	LEU	835	10.235	51.086	37.376
1519	CD2	LEU	835	12.499	51.831	37.961
1520	N	ARG	836	10.023	52.977	42.394
1521	CA	ARG	836	9.092	53.097	43.507
1522	HN	ARG	836	10.136	53.755	41.776
1523	C	ARG	836	7.993	52.055	43.370
1524	O	ARG	836	7.441	51.575	44.364
1525	CB	ARG	836	8.509	54.537	43.522
1526	CG	ARG	836	9.557	55.664	43.719
1527	CD	ARG	836	8.913	57.007	44.087
1528	NE	ARG	836	9.936	58.073	43.933
1529	CZ	ARG	836	9.751	59.361	44.190
1530	NH1	ARG	836	8.635	59.870	44.622
1531	1HH1	ARG	836	7.901	59.173	44.750
1532	2HH1	ARG	836	8.615	60.875	44.783
1533	NH2	ARG	836	10.745	60.153	43.998
1534	1HH2	ARG	836	11.571	59.655	43.659
1535	2HH2	ARG	836	10.609	61.143	44.190
1536	HE	ARG	836	10.841	57.796	43.608
1537	N	SER	837	7.685	51.710	42.124
1538	CA	SER	837	6.638	50.742	41.831
1539	HN	SER	837	8.187	52.127	41.367
1540	C	SER	837	7.219	49.524	41.124

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1541	O	SER	837	6.549	48.918	40.287
1542	CB	SER	837	5.578	51.392	40.941
1543	OG	SER	837	5.265	52.742	41.226
1544	HG	SER	837	6.121	53.196	41.183
1545	N	GLN	838	8.456	49.178	41.466
1546	CA	GLN	838	9.150	48.037	40.861
1547	HN	GLN	838	8.931	49.716	42.162
1548	C	GLN	838	8.192	46.878	40.678
1549	O	GLN	838	8.146	46.245	39.621
1550	CB	GLN	838	10.317	47.597	41.749
1551	CG	GLN	838	11.126	46.435	41.192
1552	CD	GLN	838	11.754	46.736	39.838
1553	OE1	GLN	838	12.593	47.637	39.708
1554	NE2	GLN	838	11.300	46.051	38.710
1555	1HE2	GLN	838	11.713	46.227	37.810
1556	2HE2	GLN	838	10.698	45.239	38.819
1557	N	THR	839	7.428	46.617	41.721
1558	CA	THR	839	6.438	45.559	41.743
1559	HN	THR	839	7.538	47.180	42.541
1560	C	THR	839	5.617	45.521	40.432
1561	O	THR	839	5.665	44.542	39.674
1562	CB	THR	839	5.497	45.756	42.980
1563	OG1	THR	839	5.245	47.137	43.199
1564	HG1	THR	839	4.610	47.182	43.920
1565	CG2	THR	839	6.029	45.240	44.334
1566	N	GLN	840	4.911	46.618	40.171
1567	CA	GLN	840	4.043	46.821	39.000
1568	HN	GLN	840	4.977	47.370	40.826
1569	C	GLN	840	4.787	46.827	37.655
1570	O	GLN	840	4.284	46.363	36.626
1571	CB	GLN	840	3.285	48.149	39.220
1572	CG	GLN	840	1.744	48.117	38.951
1573	CD	GLN	840	1.057	49.370	38.395
1574	OE1	GLN	840	-0.136	49.373	38.136
1575	NE2	GLN	840	1.756	50.454	38.169
1576	2HE2	GLN	840	2.758	50.364	38.342
1577	1HE2	GLN	840	1.235	51.221	37.739
1578	N	PHE	841	5.974	47.402	37.672
1579	CA	PHE	841	6.803	47.466	36.494
1580	HN	PHE	841	6.308	47.805	38.525
1581	C	PHE	841	6.951	46.051	35.974
1582	O	PHE	841	6.586	45.728	34.845
1583	CB	PHE	841	8.162	47.986	36.894
1584	CG	PHE	841	9.121	48.038	35.779
1585	CD1	PHE	841	9.173	49.152	34.962
1586	CE1	PHE	841	10.054	49.210	33.908
1587	CZ	PHE	841	10.896	48.134	33.652
1588	CE2	PHE	841	10.852	47.007	34.469
1589	CD2	PHE	841	9.958	46.962	35.523
1590	N	GLU	842	7.494	45.200	36.835
1591	CA	GLU	842	7.725	43.824	36.478
1592	HN	GLU	842	7.747	45.520	37.748
1593	C	GLU	842	6.457	43.114	36.085
1594	O	GLU	842	6.497	42.067	35.439
1595	CB	GLU	842	8.446	43.090	37.643

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1596	CG	GLU	842	9.948	43.446	37.896
1597	CD	GLU	842	10.807	43.863	36.699
1598	OE1	GLU	842	11.982	44.190	36.805
1599	OE2	GLU	842	10.143	43.835	35.511
1600	HE2	GLU	842	10.726	44.102	34.817
1601	N	GLU	843	5.323	43.685	36.452
1602	CA	GLU	843	4.073	43.059	36.084
1603	HN	GLU	843	5.329	44.536	36.976
1604	C	GLU	843	3.717	43.494	34.675
1605	O	GLU	843	3.334	42.673	33.831
1606	CB	GLU	843	2.973	43.475	37.028
1607	CG	GLU	843	1.740	42.656	36.823
1608	CD	GLU	843	0.550	43.287	37.463
1609	OE1	GLU	843	0.751	44.057	38.432
1610	OE2	GLU	843	-0.579	43.009	37.001
1611	HE2	GLU	843	-1.243	43.470	37.492
1612	N	MET	844	3.845	44.792	34.429
1613	CA	MET	844	3.554	45.353	33.128
1614	HN	MET	844	4.151	45.398	35.162
1615	C	MET	844	4.558	44.789	32.155
1616	O	MET	844	4.191	44.248	31.119
1617	CB	MET	844	3.648	46.902	33.186
1618	CG	MET	844	2.579	47.610	34.044
1619	SD	MET	844	2.732	49.395	33.860
1620	CE	MET	844	1.675	49.895	35.225
1621	N	ARG	845	5.831	44.879	32.504
1622	CA	ARG	845	6.858	44.348	31.632
1623	HN	ARG	845	6.083	45.314	33.368
1624	C	ARG	845	6.663	42.886	31.230
1625	O	ARG	845	7.031	42.498	30.125
1626	CB	ARG	845	8.222	44.487	32.276
1627	CG	ARG	845	9.338	43.990	31.382
1628	CD	ARG	845	10.592	44.687	31.817
1629	NE	ARG	845	11.788	44.423	31.025
1630	CZ	ARG	845	12.240	43.213	30.720
1631	NH1	ARG	845	11.722	42.067	31.237
1632	1HH1	ARG	845	12.111	41.185	30.975
1633	2HH1	ARG	845	10.954	42.117	31.874
1634	NH2	ARG	845	13.301	43.102	29.867
1635	1HH2	ARG	845	13.666	42.202	29.627
1636	2HH2	ARG	845	13.711	43.925	29.480
1637	HE	ARG	845	12.304	45.210	30.686
1638	N	SER	846	6.107	42.067	32.117
1639	CA	SER	846	5.895	40.660	31.804
1640	HN	SER	846	5.830	42.421	33.011
1641	C	SER	846	4.760	40.504	30.792
1642	O	SER	846	4.808	39.640	29.913
1643	CB	SER	846	5.598	39.892	33.116
1644	OG	SER	846	5.617	38.470	32.945
1645	HG	SER	846	4.910	38.245	32.334
1646	N	SER	847	3.741	41.353	30.925
1647	CA	SER	847	2.576	41.314	30.040
1648	HN	SER	847	3.773	42.038	31.653
1649	C	SER	847	2.939	41.645	28.607
1650	O	SER	847	2.409	41.039	27.664

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1651	CB	SER	847	1.478	42.262	30.584
1652	OG	SER	847	1.254	42.106	31.989
1653	HG	SER	847	0.935	41.211	32.132
1654	N	TYR	848	3.812	42.633	28.428
1655	CA	TYR	848	4.213	42.934	27.078
1656	HN	TYR	848	4.177	43.149	29.204
1657	C	TYR	848	5.231	41.906	26.606
1658	O	TYR	848	5.482	41.819	25.421
1659	CB	TYR	848	4.743	44.368	26.937
1660	CG	TYR	848	3.625	45.390	27.002
1661	CD1	TYR	848	2.598	45.389	26.052
1662	CE1	TYR	848	1.491	46.230	26.193
1663	CZ	TYR	848	1.411	47.080	27.284
1664	OH	TYR	848	0.360	47.950	27.408
1665	HH	TYR	848	0.446	48.416	28.251
1666	CE2	TYR	848	2.427	47.107	28.224
1667	CD2	TYR	848	3.523	46.270	28.079
1668	N	ILE	849	5.829	41.107	27.485
1669	CA	ILE	849	6.748	40.123	26.919
1670	HN	ILE	849	5.659	41.174	28.468
1671	C	ILE	849	5.925	39.010	26.292
1672	O	ILE	849	6.310	38.445	25.274
1673	CB	ILE	849	7.733	39.512	27.935
1674	CG2	ILE	849	8.465	38.324	27.285
1675	CG1	ILE	849	8.770	40.563	28.335
1676	CD1	ILE	849	9.397	40.319	29.678
1677	N	ARG	850	4.782	38.702	26.894
1678	CA	ARG	850	3.921	37.672	26.337
1679	HN	ARG	850	4.514	39.179	27.732
1680	C	ARG	850	3.174	38.282	25.150
1681	O	ARG	850	2.782	37.583	24.217
1682	CB	ARG	850	2.936	37.158	27.424
1683	CG	ARG	850	3.598	36.378	28.590
1684	CD	ARG	850	2.667	36.225	29.799
1685	NE	ARG	850	3.213	35.160	30.678
1686	CZ	ARG	850	2.596	34.636	31.729
1687	NH1	ARG	850	1.411	34.988	32.134
1688	1HH1	ARG	850	0.990	35.715	31.555
1689	2HH1	ARG	850	1.042	34.513	32.955
1690	NH2	ARG	850	3.215	33.722	32.386
1691	1HH2	ARG	850	4.134	33.521	31.987
1692	2HH2	ARG	850	2.749	33.318	33.196
1693	HE	ARG	850	4.123	34.807	30.459
1694	N	GLU	851	2.986	39.594	25.194
1695	CA	GLU	851	2.315	40.291	24.115
1696	HN	GLU	851	3.313	40.111	25.985
1697	C	GLU	851	3.224	40.145	22.892
1698	O	GLU	851	2.748	40.020	21.757
1699	CB	GLU	851	2.129	41.756	24.506
1700	CG	GLU	851	0.878	42.449	23.947
1701	CD	GLU	851	-0.362	41.556	23.874
1702	OE1	GLU	851	-0.767	40.962	24.903
1703	OE2	GLU	851	-0.936	41.463	22.763
1704	HE2	GLU	851	-1.682	40.889	22.840
1705	N	LEU	852	4.536	40.143	23.135

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1706	CA	LEU	852	5.503	39.980	22.058
1707	HN	LEU	852	4.861	40.255	24.074
1708	C	LEU	852	5.325	38.560	21.578
1709	O	LEU	852	5.338	38.275	20.384
1710	CB	LEU	852	6.946	40.169	22.549
1711	CG	LEU	852	7.938	39.886	21.417
1712	CD1	LEU	852	7.511	40.699	20.219
1713	CD2	LEU	852	9.362	40.214	21.805
1714	N	ILE	853	5.141	37.669	22.539
1715	CA	ILE	853	4.962	36.263	22.235
1716	HN	ILE	853	5.124	37.971	23.492
1717	C	ILE	853	3.814	35.945	21.293
1718	O	ILE	853	3.991	35.179	20.350
1719	CB	ILE	853	4.851	35.456	23.593
1720	CG1	ILE	853	5.959	35.789	24.642
1721	CG2	ILE	853	4.837	33.910	23.378
1722	CD1	ILE	853	5.707	35.276	26.075
1723	N	LYS	854	2.640	36.517	21.558
1724	CA	LYS	854	1.457	36.297	20.722
1725	HN	LYS	854	2.564	37.116	22.355
1726	C	LYS	854	1.677	36.840	19.320
1727	O	LYS	854	1.331	36.197	18.326
1728	CB	LYS	854	0.262	37.026	21.293
1729	CG	LYS	854	-0.140	36.604	22.653
1730	CD	LYS	854	-1.219	37.528	23.151
1731	CE	LYS	854	-2.034	36.824	24.193
1732	NZ	LYS	854	-3.153	37.678	24.762
1733	HZ1	LYS	854	-2.861	38.666	24.773
1734	HZ2	LYS	854	-3.995	37.577	24.176
1735	HZ3	LYS	854	-3.360	37.381	25.694
1736	N	ALA	855	2.213	38.053	19.254
1737	CA	ALA	855	2.476	38.694	17.985
1738	HN	ALA	855	2.441	38.534	20.101
1739	C	ALA	855	3.331	37.722	17.193
1740	O	ALA	855	3.093	37.505	16.007
1741	CB	ALA	855	3.210	40.003	18.197
1742	N	ILE	856	4.317	37.130	17.862
1743	CA	ILE	856	5.197	36.165	17.212
1744	HN	ILE	856	4.457	37.350	18.827
1745	C	ILE	856	4.440	34.939	16.681
1746	O	ILE	856	4.599	34.576	15.516
1747	CB	ILE	856	6.305	35.673	18.167
1748	CG2	ILE	856	7.024	34.482	17.547
1749	CG1	ILE	856	7.295	36.803	18.451
1750	CD1	ILE	856	8.262	36.508	19.591
1751	N	GLY	857	3.624	34.300	17.528
1752	CA	GLY	857	2.865	33.114	17.116
1753	HN	GLY	857	3.529	34.639	18.464
1754	C	GLY	857	1.853	33.364	16.013
1755	O	GLY	857	1.584	32.470	15.219
1756	N	LEU	858	1.272	34.561	15.966
1757	CA	LEU	858	0.266	34.833	14.952
1758	HN	LEU	858	1.526	35.269	16.625
1759	C	LEU	858	0.809	35.417	13.651
1760	O	LEU	858	0.067	36.025	12.892

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1761	CB	LEU	858	-0.852	35.738	15.543
1762	CG	LEU	858	-0.935	37.210	15.057
1763	CD1	LEU	858	-2.282	37.825	15.463
1764	CD2	LEU	858	0.214	38.078	15.593
1765	N	ARG	859	2.093	35.212	13.370
1766	CA	ARG	859	2.681	35.753	12.142
1767	HN	ARG	859	2.660	34.683	14.001
1768	C	ARG	859	3.342	34.641	11.356
1769	O	ARG	859	3.279	34.579	10.126
1770	CB	ARG	859	3.756	36.799	12.482
1771	CG	ARG	859	4.482	37.395	11.260
1772	CD	ARG	859	5.850	38.007	11.619
1773	NE	ARG	859	6.988	37.182	11.200
1774	CZ	ARG	859	7.594	37.268	10.015
1775	NH1	ARG	859	7.225	38.168	9.054
1776	1HH1	ARG	859	7.713	38.187	8.184
1777	2HH1	ARG	859	6.471	38.798	9.231
1778	NH2	ARG	859	8.627	36.413	9.759
1779	1HH2	ARG	859	9.108	36.443	8.885
1780	2HH2	ARG	859	8.889	35.748	10.461
1781	HE	ARG	859	7.335	36.506	11.850
1782	N	GLN	860	3.975	33.764	12.123
1783	CA	GLN	860	4.743	32.640	11.628
1784	HN	GLN	860	3.918	33.887	13.114
1785	C	GLN	860	4.039	31.621	10.739
1786	O	GLN	860	3.938	31.802	9.526
1787	CB	GLN	860	5.410	31.950	12.839
1788	CG	GLN	860	6.972	31.872	12.816
1789	CD	GLN	860	7.777	33.116	12.418
1790	OE1	GLN	860	7.604	34.186	12.980
1791	NE2	GLN	860	8.648	33.046	11.444
1792	2HE2	GLN	860	8.695	32.143	10.970
1793	1HE2	GLN	860	9.093	33.933	11.199
1794	N	LYS	861	3.545	30.551	11.345
1795	CA	LYS	861	2.923	29.508	10.561
1796	HN	LYS	861	3.601	30.466	12.339
1797	C	LYS	861	3.910	28.361	10.659
1798	O	LYS	861	4.792	28.191	9.811
1799	CB	LYS	861	2.682	29.908	9.079
1800	CG	LYS	861	2.106	28.758	8.216
1801	CD	LYS	861	1.917	29.096	6.735
1802	CE	LYS	861	1.412	27.852	5.992
1803	NZ	LYS	861	1.065	28.215	4.607
1804	HZ2	LYS	861	1.724	28.911	4.239
1805	HZ1	LYS	861	1.128	27.405	3.982
1806	HZ3	LYS	861	0.136	28.585	4.582
1807	N	GLY	862	3.755	27.613	11.746
1808	CA	GLY	862	4.564	26.452	12.119
1809	HN	GLY	862	3.015	27.868	12.368
1810	C	GLY	862	4.598	26.516	13.654
1811	O	GLY	862	3.551	26.710	14.274
1812	N	VAL	863	5.763	26.372	14.275
1813	CA	VAL	863	5.831	26.436	15.736
1814	HN	VAL	863	6.596	26.219	13.743
1815	C	VAL	863	7.207	26.150	16.311

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1816	O	VAL	863	7.451	26.398	17.495
1817	CB	VAL	863	4.749	25.470	16.363
1818	CG1	VAL	863	3.432	26.135	16.853
1819	CG2	VAL	863	4.303	24.329	15.418
1820	N	VAL	864	8.105	25.606	15.502
1821	CA	VAL	864	9.441	25.356	16.017
1822	HN	VAL	864	7.868	25.372	14.559
1823	C	VAL	864	10.214	26.642	15.778
1824	O	VAL	864	11.168	26.958	16.493
1825	CB	VAL	864	10.130	24.141	15.277
1826	CG1	VAL	864	10.576	24.390	13.809
1827	CG2	VAL	864	11.387	23.598	15.999
1828	N	SER	865	9.787	27.400	14.773
1829	CA	SER	865	10.446	28.656	14.481
1830	HN	SER	865	9.010	27.103	14.218
1831	C	SER	865	9.822	29.736	15.357
1832	O	SER	865	10.123	30.918	15.207
1833	CB	SER	865	10.338	29.008	12.977
1834	OG	SER	865	8.993	29.271	12.561
1835	HG	SER	865	8.491	28.461	12.687
1836	N	SER	866	8.965	29.326	16.289
1837	CA	SER	866	8.349	30.300	17.178
1838	HN	SER	866	8.747	28.354	16.378
1839	C	SER	866	9.238	30.709	18.333
1840	O	SER	866	9.409	31.901	18.572
1841	CB	SER	866	6.966	29.807	17.672
1842	OG	SER	866	5.888	30.247	16.838
1843	HG	SER	866	5.865	31.207	16.881
1844	N	SER	867	9.809	29.754	19.059
1845	CA	SER	867	10.722	30.160	20.111
1846	HN	SER	867	9.617	28.788	18.886
1847	C	SER	867	11.947	30.685	19.428
1848	O	SER	867	12.641	31.546	19.946
1849	CB	SER	867	11.053	28.960	21.034
1850	OG	SER	867	9.995	28.652	21.947
1851	HG	SER	867	9.881	29.413	22.523
1852	N	GLN	868	12.253	30.159	18.260
1853	CA	GLN	868	13.429	30.674	17.628
1854	HN	GLN	868	11.696	29.443	17.839
1855	C	GLN	868	13.229	32.139	17.268
1856	O	GLN	868	14.184	32.906	17.281
1857	CB	GLN	868	13.782	29.864	16.398
1858	CG	GLN	868	15.120	30.259	15.832
1859	CD	GLN	868	15.367	29.609	14.501
1860	OE1	GLN	868	16.487	29.631	13.990
1861	NE2	GLN	868	14.293	29.030	13.788
1862	1HE2	GLN	868	14.473	28.624	12.884
1863	2HE2	GLN	868	13.386	28.925	14.210
1864	N	ARG	869	11.988	32.524	16.962
1865	CA	ARG	869	11.656	33.911	16.585
1866	HN	ARG	869	11.254	31.846	16.990
1867	C	ARG	869	11.888	34.813	17.795
1868	O	ARG	869	12.635	35.796	17.748
1869	CB	ARG	869	10.184	33.966	16.157
1870	CG	ARG	869	9.698	35.261	15.556

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1871	CD	ARG	869	10.351	35.566	14.227
1872	NE	ARG	869	9.769	36.777	13.671
1873	CZ	ARG	869	10.332	37.527	12.738
1874	NH1	ARG	869	11.508	37.098	12.207
1875	1HH1	ARG	869	11.954	37.643	11.499
1876	2HH1	ARG	869	11.914	36.244	12.526
1877	NH2	ARG	869	9.731	38.655	12.360
1878	1HH2	ARG	869	10.147	39.221	11.648
1879	2HH2	ARG	869	8.870	38.930	12.797
1880	HE	ARG	869	8.876	37.064	14.019
1881	N	PHE	870	11.216	34.450	18.875
1882	CA	PHE	870	11.306	35.136	20.138
1883	HN	PHE	870	10.612	33.655	18.811
1884	C	PHE	870	12.763	35.347	20.485
1885	O	PHE	870	13.213	36.472	20.731
1886	CB	PHE	870	10.664	34.278	21.208
1887	CG	PHE	870	10.554	34.946	22.519
1888	CD1	PHE	870	9.942	36.188	22.618
1889	CE1	PHE	870	9.787	36.809	23.842
1890	CZ	PHE	870	10.246	36.185	24.997
1891	CE2	PHE	870	10.864	34.944	24.911
1892	CD2	PHE	870	11.014	34.328	23.668
1893	N	TYR	871	13.497	34.247	20.513
1894	CA	TYR	871	14.903	34.289	20.828
1895	HN	TYR	871	13.067	33.367	20.311
1896	C	TYR	871	15.591	35.350	19.966
1897	O	TYR	871	16.340	36.174	20.483
1898	CB	TYR	871	15.511	32.908	20.612
1899	CG	TYR	871	16.992	32.859	20.832
1900	CD1	TYR	871	17.532	32.722	22.110
1901	CE1	TYR	871	18.910	32.720	22.307
1902	CZ	TYR	871	19.747	32.857	21.210
1903	OH	TYR	871	21.112	32.882	21.399
1904	HH	TYR	871	21.530	32.623	20.569
1905	CE2	TYR	871	19.221	32.991	19.936
1906	CD2	TYR	871	17.858	32.988	19.756
1907	N	GLN	872	15.322	35.361	18.668
1908	CA	GLN	872	15.950	36.355	17.800
1909	HN	GLN	872	14.689	34.689	18.283
1910	C	GLN	872	15.405	37.765	18.019
1911	O	GLN	872	16.168	38.739	18.044
1912	CB	GLN	872	15.752	36.015	16.334
1913	CG	GLN	872	16.086	34.612	15.954
1914	CD	GLN	872	15.869	34.395	14.479
1915	OE1	GLN	872	14.744	34.153	14.025
1916	NE2	GLN	872	17.014	34.493	13.651
1917	1HE2	GLN	872	16.916	34.308	12.664
1918	2HE2	GLN	872	17.927	34.643	14.051
1919	N	LEU	873	14.087	37.895	18.144
1920	CA	LEU	873	13.550	39.228	18.350
1921	HN	LEU	873	13.484	37.099	18.097
1922	C	LEU	873	14.160	39.797	19.635
1923	O	LEU	873	14.722	40.892	19.626
1924	CB	LEU	873	12.014	39.207	18.390
1925	CG	LEU	873	11.357	38.916	17.031

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				9.854	39.038	17.129
	1926	CD1	LEU	873	11.877	39.897
	1927	CD2	LEU	873	14.099	39.033
5	1928	N	THR	874	14.656	39.500
	1929	CA	THR	874	13.668	38.132
	1930	HN	THR	874	16.176	39.693
	1931	C	THR	874	16.755	40.269
	1932	O	THR	874	14.289	38.558
	1933	CB	THR	874	14.757	37.228
10	1934	OG1	THR	874	14.602	36.794
	1935	HG1	THR	874	12.779	38.552
	1936	CG2	THR	874	16.830	39.216
	1937	N	LYS	875	18.270	39.397
	1938	CA	LYS	875	16.336	38.737
15	1939	HN	LYS	875	18.456	40.826
	1940	C	LYS	875	19.326	41.553
	1941	O	LYS	875	18.892	38.425
	1942	CB	LYS	875	20.365	38.109
	1943	CG	LYS	875	20.502	37.119
	1944	CD	LYS	875	21.960	36.934
20	1945	CE	LYS	875	22.157	35.824
	1946	NZ	LYS	875	21.494	35.952
	1947	HZ1	LYS	875	21.990	34.911
	1948	HZ2	LYS	875	23.093	35.856
	1949	HZ3	LYS	875	17.603	41.223
25	1950	N	LEU	876	17.636	42.566
	1951	CA	LEU	876	16.918	40.577
	1952	HN	LEU	876	17.397	43.581
	1953	C	LEU	876	18.051	44.628
	1954	O	LEU	876	16.554	42.714
30	1955	CB	LEU	876	16.934	43.629
	1956	CG	LEU	876	15.660	44.226
	1957	CD1	LEU	876	17.893	44.732
	1958	CD2	LEU	876	16.452	43.267
	1959	N	LEU	877	16.140	44.140
35	1960	CA	LEU	877	15.944	42.412
	1961	HN	LEU	877	17.380	44.403
	1962	C	LEU	877	17.777	45.549
	1963	O	LEU	877	15.043	43.515
	1964	CB	LEU	877	13.715	43.547
	1965	CG	LEU	877	12.588	43.029
40	1966	CD1	LEU	877	13.447	44.988
	1967	CD2	LEU	877	18.000	43.343
	1968	N	ASP	878	19.198	43.467
	1969	CA	ASP	878	17.635	42.432
45	1970	HN	ASP	878	20.328	44.239
	1971	C	ASP	878	21.123	44.895
	1972	O	ASP	878	19.733	42.092
	1973	CB	ASP	878	18.831	41.367
	1974	CG	ASP	878	17.986	42.034
	1975	OD1	ASP	878	18.972	40.138
50	1976	OD2	ASP	878	18.343	39.811
	1977	HD2	ASP	878	20.400	44.149
	1978	N	ASN	879	21.459	44.813
	1979	CA	ASN	879	19.715	43.614
	1980	HN	ASN	879		21.657

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1981	C	ASN	879	21.137	46.275	21.164
1982	O	ASN	879	21.914	47.011	20.551
1983	CB	ASN	879	21.683	44.063	20.066
1984	CG	ASN	879	21.183	44.755	18.793
1985	OD1	ASN	879	21.933	45.363	18.044
1986	ND2	ASN	879	19.908	44.712	18.513
1987	1HD2	ASN	879	19.659	45.328	17.734
1988	2HD2	ASN	879	19.297	44.276	19.204
1989	N	LEU	880	19.975	46.683	21.653
1990	CA	LEU	880	19.505	48.049	21.499
1991	HN	LEU	880	19.402	46.028	22.145
1992	C	LEU	880	20.218	48.908	22.537
1993	O	LEU	880	20.382	50.115	22.363
1994	CB	LEU	880	17.967	48.063	21.730
1995	CG	LEU	880	17.118	49.090	20.933
1996	CD1	LEU	880	17.370	48.929	19.428
1997	CD2	LEU	880	15.612	48.968	21.222
1998	N	HIS	881	20.637	48.265	23.626
1999	CA	HIS	881	21.366	48.965	24.663
2000	HN	HIS	881	20.445	47.289	23.728
2001	C	HIS	881	22.677	49.372	24.018
2002	O	HIS	881	23.069	50.525	24.094
2003	CB	HIS	881	21.625	48.058	25.868
2004	CG	HIS	881	20.434	47.892	26.767
2005	ND1	HIS	881	19.932	46.661	27.114
2006	CE1	HIS	881	18.881	46.823	27.903
2007	NE2	HIS	881	18.691	48.114	28.080
2008	HE2	HIS	881	17.945	48.535	28.652
2009	CD2	HIS	881	19.648	48.811	27.381
2010	N	ASP	882	23.343	48.454	23.333
2011	CA	ASP	882	24.594	48.867	22.735
2012	HN	ASP	882	22.998	47.520	23.234
2013	C	ASP	882	24.485	49.904	21.618
2014	O	ASP	882	25.405	50.714	21.471
2015	CB	ASP	882	25.429	47.634	22.300
2016	CG	ASP	882	26.949	47.831	22.199
2017	OD1	ASP	882	27.668	47.123	21.510
2018	OD2	ASP	882	27.396	48.890	22.939
2019	HD2	ASP	882	28.333	48.968	22.844
2020	N	LEU	883	23.418	49.918	20.817
2021	CA	LEU	883	23.396	50.978	19.804
2022	HN	LEU	883	22.680	49.249	20.903
2023	C	LEU	883	23.025	52.309	20.464
2024	O	LEU	883	23.535	53.352	20.062
2025	CB	LEU	883	22.497	50.703	18.565
2026	CG	LEU	883	21.601	49.435	18.580
2027	CD1	LEU	883	20.880	49.283	17.233
2028	CD2	LEU	883	22.390	48.153	18.893
2029	N	VAL	884	22.176	52.274	21.495
2030	CA	VAL	884	21.806	53.511	22.196
2031	HN	VAL	884	21.791	51.400	21.791
2032	C	VAL	884	23.037	54.118	22.876
2033	O	VAL	884	23.216	55.331	22.884
2034	CB	VAL	884	20.666	53.265	23.239
2035	CG1	VAL	884	20.883	54.102	24.501

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2036	CG2	VAL	884	19.337	53.649	22.622
2037	N	LYS	885	23.896	53.278	23.440
2038	CA	LYS	885	25.100	53.795	24.070
2039	HN	LYS	885	23.716	52.295	23.431
2040	C	LYS	885	25.856	54.646	23.041
2041	O	LYS	885	26.084	55.831	23.258
2042	CB	LYS	885	25.988	52.630	24.587
2043	CG	LYS	885	27.187	53.104	25.445
2044	CD	LYS	885	27.964	51.982	26.141
2045	CE	LYS	885	26.976	50.933	26.667
2046	NZ	LYS	885	27.723	49.772	27.183
2047	HZ2	LYS	885	28.586	50.074	27.649
2048	HZ1	LYS	885	27.181	49.264	27.889
2049	HZ3	LYS	885	27.946	49.156	26.427
2050	N	GLN	886	26.216	54.045	21.909
2051	CA	GLN	886	26.945	54.767	20.866
2052	HN	GLN	886	25.985	53.083	21.768
2053	C	GLN	886	26.165	55.928	20.329
2054	O	GLN	886	26.734	56.902	19.834
2055	CB	GLN	886	27.349	53.800	19.732
2056	CG	GLN	886	28.246	52.587	20.145
2057	CD	GLN	886	28.640	51.552	19.083
2058	OE1	GLN	886	29.370	50.614	19.358
2059	NE2	GLN	886	28.212	51.682	17.853
2060	2HE2	GLN	886	27.663	52.525	17.674
2061	1HE2	GLN	886	28.572	50.989	17.195
2062	N	LEU	887	24.856	55.851	20.484
2063	CA	LEU	887	24.046	56.947	20.040
2064	HN	LEU	887	24.439	55.045	20.903
2065	C	LEU	887	24.106	58.077	21.040
2066	O	LEU	887	24.103	59.242	20.645
2067	CB	LEU	887	22.623	56.496	19.816
2068	CG	LEU	887	22.595	56.012	18.381
2069	CD1	LEU	887	21.174	55.720	18.026
2070	CD2	LEU	887	23.193	57.071	17.439
2071	N	HIS	888	24.181	57.749	22.328
2072	CA	HIS	888	24.263	58.786	23.357
2073	HN	HIS	888	24.182	56.786	22.595
2074	C	HIS	888	25.637	59.455	23.422
2075	O	HIS	888	25.708	60.682	23.529
2076	CB	HIS	888	23.881	58.215	24.732
2077	CG	HIS	888	22.409	57.945	24.848
2078	ND1	HIS	888	21.777	57.315	25.917
2079	CE1	HIS	888	20.502	57.354	25.486
2080	NE2	HIS	888	20.251	57.923	24.276
2081	CD2	HIS	888	21.500	58.309	23.864
2082	HE2	HIS	888	19.352	58.041	23.788
2083	N	LEU	889	26.721	58.682	23.357
2084	CA	LEU	889	28.044	59.302	23.396
2085	HN	LEU	889	26.630	57.688	23.284
2086	C	LEU	889	28.165	60.488	22.389
2087	O	LEU	889	28.636	61.533	22.815
2088	CB	LEU	889	29.181	58.264	23.171
2089	CG	LEU	889	29.449	57.220	24.288
2090	CD1	LEU	889	28.805	57.678	25.604

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2091	CD2	LEU	889	28.940	55.816	23.924
2092	N	TYR	890	27.761	60.362	21.102
2093	CA	TYR	890	27.894	61.500	20.123
2094	HN	TYR	890	27.367	59.496	20.795
2095	C	TYR	890	27.006	62.611	20.566
2096	O	TYR	890	27.299	63.777	20.356
2097	CB	TYR	890	27.462	61.227	18.625
2098	CG	TYR	890	28.164	62.223	17.650
2099	CD1	TYR	890	27.744	62.487	16.309
2100	CE1	TYR	890	28.494	63.375	15.472
2101	CZ	TYR	890	29.624	63.996	16.007
2102	OH	TYR	890	30.353	64.863	15.221
2103	HH	TYR	890	31.162	65.093	15.692
2104	CE2	TYR	890	30.014	63.735	17.301
2105	CD2	TYR	890	29.297	62.872	18.095
2106	N	CYS	891	25.909	62.247	21.191
2107	CA	CYS	891	24.971	63.257	21.570
2108	HN	CYS	891	25.735	61.284	21.397
2109	C	CYS	891	25.411	64.088	22.743
2110	O	CYS	891	25.410	65.316	22.669
2111	CB	CYS	891	23.625	62.607	21.821
2112	SG	CYS	891	22.292	63.762	22.287
2113	HG	CYS	891	21.160	63.081	22.481
2114	N	LEU	892	25.787	63.431	23.828
2115	CA	LEU	892	26.231	64.187	24.975
2116	HN	LEU	892	25.765	62.431	23.853
2117	C	LEU	892	27.389	65.064	24.502
2118	O	LEU	892	27.345	66.291	24.619
2119	CB	LEU	892	26.689	63.226	26.109
2120	CG	LEU	892	25.609	62.364	26.818
2121	CD1	LEU	892	24.209	62.911	26.506
2122	CD2	LEU	892	25.683	60.879	26.427
2123	N	ASN	893	28.404	64.415	23.941
2124	CA	ASN	893	29.581	65.087	23.411
2125	HN	ASN	893	28.358	63.418	23.880
2126	C	ASN	893	29.097	66.302	22.642
2127	O	ASN	893	29.026	67.386	23.195
2128	CB	ASN	893	30.335	64.103	22.470
2129	CG	ASN	893	31.777	64.465	22.099
2130	OD1	ASN	893	32.504	63.700	21.483
2131	ND2	ASN	893	32.252	65.622	22.475
2132	1HD2	ASN	893	33.260	65.701	22.314
2133	2HD2	ASN	893	31.652	66.199	23.065
2134	N	THR	894	28.741	66.123	21.377
2135	CA	THR	894	28.254	67.246	20.590
2136	HN	THR	894	28.807	65.215	20.963
2137	C	THR	894	27.525	68.300	21.446
2138	O	THR	894	27.814	69.494	21.339
2139	CB	THR	894	27.345	66.758	19.467
2140	OG1	THR	894	26.339	65.975	20.047
2141	HG1	THR	894	26.534	65.064	19.806
2142	CG2	THR	894	28.154	66.447	18.220
2143	N	PHE	895	26.618	67.870	22.315
2144	CA	PHE	895	25.882	68.810	23.169
2145	HN	PHE	895	26.433	66.890	22.389

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2146	C	PHE	895	26.754	69.636	24.119
2147	O	PHE	895	26.385	70.750	24.493
2148	CB	PHE	895	24.841	68.056	23.988
2149	CG	PHE	895	24.061	68.928	24.928
2150	CD1	PHE	895	22.887	69.546	24.518
2151	CE1	PHE	895	22.143	70.328	25.391
2152	CZ	PHE	895	22.575	70.502	26.697
2153	CE2	PHE	895	23.753	69.892	27.118
2154	CD2	PHE	895	24.488	69.112	26.237
2155	N	ILE	896	27.893	69.086	24.527
2156	CA	ILE	896	28.794	69.797	25.426
2157	HN	ILE	896	28.136	68.169	24.212
2158	C	ILE	896	30.000	70.348	24.666
2159	O	ILE	896	31.141	70.250	25.129
2160	CB	ILE	896	29.230	68.835	26.605
2161	CG1	ILE	896	28.050	68.095	27.313
2162	CG2	ILE	896	30.071	69.563	27.700
2163	CD1	ILE	896	28.438	67.191	28.501
2164	N	GLN	897	29.736	70.910	23.488
2165	CA	GLN	897	30.771	71.515	22.651
2166	HN	GLN	897	28.791	70.918	23.162
2167	C	GLN	897	30.118	72.518	21.717
2168	O	GLN	897	29.586	72.138	20.671
2169	CB	GLN	897	31.527	70.428	21.855
2170	CG	GLN	897	32.767	70.911	21.033
2171	CD	GLN	897	33.307	70.024	19.904
2172	OE1	GLN	897	34.248	70.384	19.214
2173	NE2	GLN	897	32.742	68.872	19.651
2174	2HE2	GLN	897	31.918	68.661	20.217
2175	1HE2	GLN	897	33.120	68.374	18.843
2176	N	SER	898	27.960	71.999	21.407
2177	CA	SER	898	26.923	72.646	20.604
2178	HN	SER	898	27.704	71.536	22.256
2179	C	SER	898	27.240	74.059	20.113
2180	O	SER	898	27.020	74.369	18.946
2181	CB	SER	898	25.579	72.638	21.346
2182	OG	SER	898	25.563	73.390	22.558
2183	HG	SER	898	24.693	73.242	22.952
2184	N	ARG	899	27.753	74.924	20.980
2185	CA	ARG	899	28.055	76.278	20.534
2186	HN	ARG	899	27.929	74.649	21.925
2187	C	ARG	899	29.194	76.268	19.523
2188	O	ARG	899	29.169	77.014	18.539
2189	CB	ARG	899	28.395	77.183	21.725
2190	CG	ARG	899	27.341	77.160	22.830
2191	CD	ARG	899	25.920	77.400	22.300
2192	NE	ARG	899	25.679	78.756	21.802
2193	CZ	ARG	899	25.625	79.845	22.569
2194	NH1	ARG	899	25.713	79.793	23.932
2195	1HH1	ARG	899	25.662	80.613	24.501
2196	2HH1	ARG	899	25.777	78.923	24.416
2197	NH2	ARG	899	25.471	81.061	21.972
2198	1HH2	ARG	899	25.413	81.909	22.499
2199	2HH2	ARG	899	25.387	81.153	20.981
2200	HE	ARG	899	25.546	78.874	20.818

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2201	N	ALA	900	31.651	74.889	20.070
2202	CA	ALA	900	32.565	75.329	19.028
2203	HN	ALA	900	31.963	74.238	20.761
2204	C	ALA	900	31.840	74.738	17.822
2205	O	ALA	900	31.805	75.321	16.735
2206	CB	ALA	900	33.957	74.712	19.249
2207	N	LEU	901	31.241	73.571	18.051
2208	CA	LEU	901	30.508	72.855	17.019
2209	HN	LEU	901	31.297	73.172	18.966
2210	C	LEU	901	29.275	73.631	16.592
2211	O	LEU	901	28.923	73.650	15.414
2212	CB	LEU	901	30.124	71.437	17.530
2213	CG	LEU	901	30.236	70.247	16.538
2214	CD1	LEU	901	30.568	68.956	17.298
2215	CD2	LEU	901	28.958	70.045	15.706
2216	N	SER	902	28.605	74.242	17.558
2217	CA	SER	902	27.445	75.073	17.258
2218	HN	SER	902	28.899	74.133	18.507
2219	C	SER	902	26.110	74.426	16.874
2220	O	SER	902	25.281	75.109	16.273
2221	CB	SER	902	27.808	76.071	16.151
2222	OG	SER	902	28.887	76.954	16.451
2223	HG	SER	902	29.185	77.309	15.605
2224	N	VAL	903	25.875	73.154	17.179
2225	CA	VAL	903	24.579	72.558	16.829
2226	HN	VAL	903	26.574	72.608	17.642
2227	C	VAL	903	23.634	72.822	18.011
2228	O	VAL	903	24.083	72.826	19.154
2229	CB	VAL	903	24.709	71.008	16.548
2230	CG1	VAL	903	25.798	70.582	15.525
2231	CG2	VAL	903	24.985	70.162	17.815
2232	N	GLU	904	22.347	73.037	17.745
2233	CA	GLU	904	21.379	73.348	18.812
2234	HN	GLU	904	22.030	72.987	16.798
2235	C	GLU	904	20.246	72.324	19.082
2236	O	GLU	904	19.542	71.921	18.159
2237	CB	GLU	904	20.743	74.726	18.525
2238	CG	GLU	904	21.151	75.892	19.461
2239	CD	GLU	904	22.541	76.479	19.185
2240	OE1	GLU	904	22.754	77.073	18.098
2241	OE2	GLU	904	23.424	76.353	20.069
2242	HE2	GLU	904	24.226	76.756	19.773
2243	N	PHE	905	20.068	71.932	20.351
2244	CA	PHE	905	19.009	70.985	20.761
2245	HN	PHE	905	20.680	72.297	21.053
2246	C	PHE	905	17.830	71.786	21.373
2247	O	PHE	905	18.056	72.736	22.126
2248	CB	PHE	905	19.546	69.991	21.809
2249	CG	PHE	905	20.908	69.434	21.491
2250	CD1	PHE	905	21.053	68.195	20.896
2251	CE1	PHE	905	22.302	67.717	20.598
2252	CZ	PHE	905	23.450	68.464	20.853
2253	CE2	PHE	905	23.313	69.690	21.437
2254	CD2	PHE	905	22.044	70.175	21.759
2255	N	PRO	906	16.568	71.401	21.088

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2256	CA	PRO	906	15.415	72.135	21.630
2257	CD	PRO	906	16.114	70.141	20.461
2258	C	PRO	906	15.251	72.062	23.145
2259	O	PRO	906	16.142	71.609	23.854
2260	CB	PRO	906	14.241	71.504	20.899
2261	CG	PRO	906	14.638	70.083	20.855
2262	N	GLU	907	14.098	72.520	23.629
2263	CA	GLU	907	13.795	72.507	25.059
2264	HN	GLU	907	13.418	72.885	22.994
2265	C	GLU	907	13.842	71.099	25.612
2266	O	GLU	907	14.652	70.779	26.492
2267	CB	GLU	907	12.399	73.087	25.305
2268	CG	GLU	907	12.359	74.589	25.235
2269	CD	GLU	907	13.301	75.215	26.243
2270	OE1	GLU	907	14.508	74.896	26.220
2271	OE2	GLU	907	12.832	76.021	27.067
2272	HE2	GLU	907	13.523	76.333	27.631
2273	N	MET	908	12.948	70.271	25.087
2274	CA	MET	908	12.861	68.895	25.507
2275	HN	MET	908	12.320	70.609	24.386
2276	C	MET	908	14.249	68.252	25.562
2277	O	MET	908	14.870	68.271	26.618
2278	CB	MET	908	11.912	68.116	24.584
2279	CG	MET	908	10.604	67.677	25.273
2280	SD	MET	908	10.728	67.416	27.096
2281	CE	MET	908	11.156	65.740	27.227
2282	N	MET	909	14.758	67.722	24.452
2283	CA	MET	909	16.077	67.061	24.448
2284	HN	MET	909	14.235	67.774	23.601
2285	C	MET	909	17.170	67.737	25.237
2286	O	MET	909	18.035	67.069	25.802
2287	CB	MET	909	16.519	66.828	22.977
2288	CG	MET	909	17.899	66.165	22.784
2289	SD	MET	909	18.232	65.948	21.029
2290	CE	MET	909	19.853	65.180	21.158
2291	N	SER	910	17.158	69.058	25.252
2292	CA	SER	910	18.176	69.798	25.976
2293	HN	SER	910	16.441	69.553	24.759
2294	C	SER	910	18.197	69.481	27.480
2295	O	SER	910	19.277	69.320	28.049
2296	CB	SER	910	17.984	71.313	25.716
2297	OG	SER	910	16.821	71.846	26.359
2298	HG	SER	910	16.055	71.406	25.978
2299	N	GLU	911	17.014	69.378	28.106
2300	CA	GLU	911	16.852	69.103	29.554
2301	HN	GLU	911	16.185	69.496	27.559
2302	C	GLU	911	17.169	67.641	29.921
2303	O	GLU	911	17.828	67.362	30.929
2304	CB	GLU	911	15.399	69.460	30.000
2305	CG	GLU	911	15.156	69.773	31.529
2306	CD	GLU	911	14.687	71.232	31.813
2307	OE1	GLU	911	15.306	72.174	31.267
2308	OE2	GLU	911	13.718	71.441	32.590
2309	HE2	GLU	911	13.562	72.371	32.656
2310	N	VAL	912	16.693	66.718	29.088

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2311	CA	VAL	912	16.907	65.293	29.296
2312	HN	VAL	912	16.168	67.015	28.290
2313	C	VAL	912	18.373	64.971	29.082
2314	O	VAL	912	18.964	64.230	29.866
2315	CB	VAL	912	15.999	64.466	28.300
2316	CG1	VAL	912	14.508	64.893	28.211
2317	CG2	VAL	912	16.511	64.465	26.839
2318	N	ILE	913	18.973	65.514	28.026
2319	CA	ILE	913	20.389	65.246	27.825
2320	HN	ILE	913	18.465	66.091	27.387
2321	C	ILE	913	21.054	65.695	29.123
2322	O	ILE	913	21.556	64.862	29.876
2323	CB	ILE	913	20.963	66.006	26.611
2324	CG2	ILE	913	22.463	65.834	26.555
2325	CG1	ILE	913	20.385	65.418	25.322
2326	CD1	ILE	913	20.604	66.257	24.089
2327	N	ALA	914	21.002	67.001	29.398
2328	CA	ALA	914	21.566	67.613	30.615
2329	HN	ALA	914	20.554	67.602	28.736
2330	C	ALA	914	21.374	66.795	31.884
2331	O	ALA	914	22.286	66.672	32.706
2332	CB	ALA	914	20.967	69.026	30.719
2333	N	ALA	915	20.169	66.272	32.061
2334	CA	ALA	915	19.888	65.470	33.231
2335	HN	ALA	915	19.452	66.433	31.384
2336	C	ALA	915	20.679	64.169	33.202
2337	O	ALA	915	21.380	63.839	34.153
2338	CB	ALA	915	18.369	65.242	33.315
2339	N	GLN	916	20.582	63.445	32.093
2340	CA	GLN	916	21.263	62.164	31.955
2341	HN	GLN	916	20.028	63.787	31.334
2342	C	GLN	916	22.784	62.163	31.856
2343	O	GLN	916	23.422	61.208	32.299
2344	CB	GLN	916	20.717	61.415	30.737
2345	CG	GLN	916	19.253	61.040	30.828
2346	CD	GLN	916	18.940	60.208	32.056
2347	OE1	GLN	916	19.638	59.237	32.361
2348	NE2	GLN	916	18.007	60.708	32.969
2349	1HE2	GLN	916	17.720	60.104	33.720
2350	2HE2	GLN	916	17.531	61.588	32.810
2351	N	LEU	917	23.371	63.214	31.288
2352	CA	LEU	917	24.819	63.244	31.093
2353	HN	LEU	917	22.816	63.991	30.991
2354	C	LEU	917	25.674	62.568	32.174
2355	O	LEU	917	26.442	61.655	31.866
2356	CB	LEU	917	25.308	64.696	30.824
2357	CG	LEU	917	24.629	65.496	29.680
2358	CD1	LEU	917	25.512	65.475	28.425
2359	CD2	LEU	917	23.227	64.967	29.336
2360	N	PRO	918	25.556	62.991	33.449
2361	CA	PRO	918	26.384	62.331	34.468
2362	CD	PRO	918	24.669	63.995	34.066
2363	C	PRO	918	26.046	60.853	34.659
2364	O	PRO	918	26.772	59.978	34.194
2365	CB	PRO	918	26.109	63.164	35.722

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2366	CG	PRO	918	24.691	63.591	35.528
2367	N	LYS	919	24.927	60.589	35.323
2368	CA	LYS	919	24.463	59.233	35.620
2369	HN	LYS	919	24.371	61.358	35.638
2370	C	LYS	919	24.606	58.128	34.550
2371	O	LYS	919	24.720	56.946	34.900
2372	CB	LYS	919	22.997	59.291	36.064
2373	CG	LYS	919	22.030	59.560	34.928
2374	CD	LYS	919	20.583	59.336	35.345
2375	CE	LYS	919	20.083	60.442	36.262
2376	NZ	LYS	919	18.618	60.349	36.653
2377	HZ1	LYS	919	18.227	61.297	36.750
2378	HZ2	LYS	919	18.100	59.837	35.926
2379	HZ3	LYS	919	18.536	59.864	37.524
2380	N	ILE	920	24.591	58.493	33.265
2381	CA	ILE	920	24.699	57.512	32.172
2382	HN	ILE	920	24.503	59.463	33.038
2383	C	ILE	920	26.087	56.939	31.960
2384	O	ILE	920	26.377	55.800	32.329
2385	CB	ILE	920	24.127	58.173	30.852
2386	CG1	ILE	920	22.815	57.520	30.312
2387	CG2	ILE	920	25.168	58.202	29.690
2388	CD1	ILE	920	21.527	58.350	30.490
2389	N	LEU	921	26.923	57.761	31.330
2390	CA	LEU	921	26.299	57.423	30.985
2391	HN	LEU	921	26.586	58.668	31.076
2392	C	LEU	921	28.969	56.365	31.867
2393	O	LEU	921	29.557	55.412	31.351
2394	CB	LEU	921	29.155	58.720	30.925
2395	CG	LEU	921	29.319	59.549	32.228
2396	CD1	LEU	921	30.099	60.839	31.938
2397	CD2	LEU	921	27.973	59.894	32.886
2398	N	ALA	922	28.866	56.524	33.185
2399	CA	ALA	922	29.474	55.585	34.132
2400	HN	ALA	922	28.358	57.309	33.540
2401	C	ALA	922	28.974	54.145	33.984
2402	O	ALA	922	29.703	53.261	33.522
2403	CB	ALA	922	29.258	56.148	35.547
2404	N	GLY	923	27.727	53.925	34.405
2405	CA	GLY	923	27.115	52.605	34.341
2406	HN	GLY	923	27.198	54.688	34.776
2407	C	GLY	923	26.426	52.237	35.647
2408	O	GLY	923	26.387	51.071	36.044
2409	N	MET	924	25.866	53.251	36.308
2410	CA	MET	924	25.182	53.106	37.593
2411	HN	MET	924	25.916	54.163	35.901
2412	C	MET	924	23.656	52.955	37.392
2413	O	MET	924	22.851	53.294	38.269
2414	CB	MET	924	25.507	54.360	38.450
2415	CG	MET	924	26.778	55.139	38.049
2416	SD	MET	924	26.396	56.892	37.892
2417	CE	MET	924	26.396	57.420	37.064
2418	N	VAL	925	27.901	52.427	36.214
2419	CA	VAL	925	23.302	52.172	35.734
2420	HN	VAL	925	21.930	52.179	35.594
				24.046		

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2421	C	VAL	925	21.829	50.671	35.391
2422	O	VAL	925	22.810	50.084	34.932
2423	CB	VAL	925	21.666	53.060	34.453
2424	CG1	VAL	925	21.087	54.480	34.706
2425	CG2	VAL	925	22.920	53.281	33.574
2426	N	LYS	926	20.666	50.053	35.581
2427	CA	LYS	926	20.552	48.628	35.274
2428	HN	LYS	926	19.878	50.558	35.931
2429	C	LYS	926	19.777	48.267	34.014
2430	O	LYS	926	18.544	48.228	34.010
2431	CB	LYS	926	19.948	47.873	36.448
2432	CG	LYS	926	19.773	46.377	36.216
2433	CD	LYS	926	18.912	45.841	37.339
2434	CE	LYS	926	18.473	44.409	37.153
2435	NZ	LYS	926	17.517	43.918	38.231
2436	HZ1	LYS	926	16.988	44.716	38.611
2437	HZ2	LYS	926	16.862	43.235	37.825
2438	HZ3	LYS	926	18.038	43.483	38.966
2439	N	PRO	927	20.529	47.980	32.960
2440	CA	PRO	927	19.971	47.592	31.674
2441	C	PRO	927	19.437	46.168	31.795
2442	O	PRO	927	20.208	45.247	32.038
2443	CB	PRO	927	21.082	47.730	30.622
2444	CG	PRO	927	22.370	47.475	31.420
2445	CD	PRO	927	22.089	48.145	32.767
2446	N	LEU	928	18.132	45.976	31.641
2447	CA	LEU	928	17.573	44.628	31.718
2448	HN	LEU	928	17.530	46.756	31.472
2449	C	LEU	928	17.956	43.896	30.438
2450	O	LEU	928	17.995	44.499	29.370
2451	CB	LEU	928	16.059	44.688	31.811
2452	CG	LEU	928	15.563	45.735	32.794
2453	CD1	LEU	928	14.058	45.677	32.854
2454	CD2	LEU	928	16.163	45.484	34.161
2455	N	LEU	929	18.239	42.605	30.527
2456	CA	LEU	929	18.602	41.856	29.326
2457	HN	LEU	929	18.205	42.144	31.413
2458	C	LEU	929	17.790	40.570	29.208
2459	O	LEU	929	17.364	40.025	30.218
2460	CB	LEU	929	20.098	41.528	29.346
2461	CG	LEU	929	21.046	42.715	29.164
2462	CD1	LEU	929	22.449	42.196	28.955
2463	CD2	LEU	929	20.639	43.537	27.954
2464	N	PHE	930	17.547	40.099	27.984
2465	CA	PHE	930	16.801	38.847	27.812
2466	HN	PHE	930	17.874	40.599	27.182
2467	C	PHE	930	17.772	37.692	27.803
2468	O	PHE	930	17.483	36.618	28.320
2469	CB	PHE	930	16.012	38.831	26.509
2470	CG	PHE	930	14.783	39.658	26.558
2471	CD1	PHE	930	13.647	39.198	27.206
2472	CE1	PHE	930	12.534	40.005	27.331
2473	CZ	PHE	930	12.552	41.283	26.807
2474	CE2	PHE	930	13.680	41.743	26.155
2475	CD2	PHE	930	14.787	40.933	26.035

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2476	N	HIS	931	18.929	37.930	27.198
2477	CA	HIS	931	19.985	36.938	27.104
2478	HN	HIS	931	19.079	38.830	26.789
2479	C	HIS	931	21.218	37.571	27.755
2480	O	HIS	931	21.562	38.710	27.432
2481	CB	HIS	931	20.300	36.628	25.631
2482	CG	HIS	931	19.093	36.359	24.792
2483	ND1	HIS	931	18.209	35.328	25.058
2484	CE1	HIS	931	17.249	35.325	24.154
2485	NE2	HIS	931	17.472	36.322	23.306
2486	HE2	HIS	931	16.883	36.563	22.496
2487	CD2	HIS	931	18.612	36.976	23.686
2488	N	LYS	932	21.870	36.851	28.668
2489	CA	LYS	932	23.078	37.366	29.332
2490	HN	LYS	932	21.531	35.941	28.907
2491	C	LYS	932	24.313	36.931	28.518
2492	OXT	LYS	932	25.424	37.309	29.006
2493	O	LYS	932	24.485	35.702	28.245
2494	CB	LYS	932	23.155	36.832	30.789
2495	CG	LYS	932	23.857	35.456	30.904
2496	CD	LYS	932	25.374	35.521	31.097
2497	CE	LYS	932	25.987	34.158	30.750
2498	NZ	LYS	932	27.457	34.263	30.767
2499	HZ2	LYS	932	27.766	34.889	31.519
2500	HZ1	LYS	932	27.893	33.354	30.955
2501	HZ3	LYS	932	27.777	34.611	29.886
2502	CL1	RWJ	1	14.371	60.020	15.893
2503	C2	RWJ	1	15.944	60.715	16.157
2504	C3	RWJ	1	17.076	59.893	16.188
2505	C4	RWJ	1	16.933	58.402	15.993
2506	F5	RWJ	1	16.659	57.827	17.160
2507	F6	RWJ	1	18.068	57.907	15.510
2508	F7	RWJ	1	15.944	58.160	15.137
2509	C8	RWJ	1	18.342	60.452	16.400
2510	C9	RWJ	1	18.475	61.834	16.581
2511	C10	RWJ	1	19.813	62.425	16.805
2512	N11	RWJ	1	20.828	61.627	17.080
2513	N12	RWJ	1	22.183	62.087	17.319
2514	S13	RWJ	1	23.312	60.945	16.624
2515	O14	RWJ	1	22.844	59.613	16.851
2516	O15	RWJ	1	24.594	61.111	17.236
2517	C16	RWJ	1	23.453	61.246	14.814
2518	C17	RWJ	1	24.421	62.130	14.325
2519	C18	RWJ	1	24.528	62.358	12.948
2520	C19	RWJ	1	23.667	61.702	12.060
2521	I20	RWJ	1	23.827	62.045	9.995
2522	C21	RWJ	1	22.698	60.818	12.550
2523	C22	RWJ	1	22.591	60.589	13.927
2524	C23	RWJ	1	22.448	63.426	16.774
2525	C24	RWJ	1	23.812	63.921	17.247
2526	C25	RWJ	1	21.352	64.423	17.195
2527	C26	RWJ	1	19.977	63.923	16.713
2528	C27	RWJ	1	17.343	62.656	16.550
2529	C28	RWJ	1	16.077	62.097	16.337

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TABLE 6

SUBSET OF ATOMIC COORDINATES OF GR α IN COMPLEX WITH THE
 BENZOXAZIN-1-ONE OBTAINED FROM MODELING OF THE CRYSTAL
 STRUCTURE OF GR α IN COMPLEX WITH FP

Atom Number	Atom Type	Residue Name	Residue Number	Coordinate x	Coordinate y	Coordinate z
1	N	LEU	544	5.940	62.649	11.764
2	CA	LEU	544	5.974	64.102	11.777
3	CB	LEU	544	5.952	64.855	13.135
4	CG	LEU	544	6.701	64.350	14.406
5	CD1	LEU	544	6.322	65.241	15.616
6	CD2	LEU	544	6.415	62.880	14.786
7	C	LEU	544	7.164	64.437	10.826
8	O	LEU	544	8.239	63.851	10.879
9	HN	LEU	544	6.575	62.118	12.352
10	N	THR	556	26.585	69.651	7.255
11	CA	THR	556	26.781	68.735	8.382
12	CB	THR	556	28.265	68.599	8.879
13	OG1	THR	556	29.183	68.249	7.833
14	CG2	THR	556	28.366	67.548	10.003
15	C	THR	556	25.830	69.214	9.501
16	O	THR	556	24.880	68.495	9.743
17	HN	THR	556	27.395	69.596	6.643
18	HG1	THR	556	30.058	68.161	8.250
19	N	ILE	559	21.633	70.003	8.878
20	CA	ILE	559	20.880	68.737	8.871
21	CB	ILE	559	21.416	67.541	8.014
22	CG2	ILE	559	20.550	66.283	8.280
23	CG1	ILE	559	21.498	67.829	6.495
24	CD1	ILE	559	21.957	66.639	5.616
25	C	ILE	559	20.891	68.309	10.355
26	O	ILE	559	19.818	68.267	10.917
27	HN	ILE	559	22.559	69.900	8.462
28	N	MET	560	22.116	67.951	11.005
29	CA	MET	560	22.238	67.530	12.398
30	CB	MET	560	23.650	67.542	13.010
31	CG	MET	560	24.560	66.453	12.433
32	SD	MET	560	26.049	66.144	13.442
33	CE	MET	560	26.836	64.975	12.282
34	C	MET	560	21.376	68.480	13.244
35	O	MET	560	20.739	67.976	14.146
36	HN	MET	560	22.988	67.997	10.493
37	N	THR	562	18.442	70.366	12.296
38	CA	THR	562	16.979	69.979	12.264
39	CB	THR	562	16.011	70.077	11.038
40	OG1	THR	562	16.263	69.083	10.049
41	CG2	THR	562	15.882	71.488	10.437
42	C	THR	562	16.792	68.531	12.863
43	O	THR	562	15.662	68.207	13.197
44	HN	THR	562	18.984	70.366	11.451
45	HG1	THR	562	15.410	68.898	9.600

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46	N	LEU	563	17.916	67.661	12.989
47	CA	LEU	563	17.667	66.302	13.464
48	CB	LEU	563	18.721	65.226	13.171
49	CG	LEU	563	18.460	64.497	11.832
50	CD1	LEU	563	17.838	65.349	10.696
51	CD2	LEU	563	19.764	63.838	11.363
52	C	LEU	563	17.434	66.528	14.954
53	O	LEU	563	16.437	66.052	15.458
54	HN	LEU	563	18.676	67.802	12.334
55	N	ASN	564	18.322	67.363	15.671
56	CA	ASN	564	17.960	67.789	17.027
57	CB	ASN	564	18.861	68.818	17.707
58	CG	ASN	564	20.332	68.431	17.754
59	OD1	ASN	564	20.859	67.537	17.111
60	ND2	ASN	564	21.098	69.270	18.563
61	C	ASN	564	16.512	68.379	17.099
62	O	ASN	564	15.949	68.320	18.183
63	HN	ASN	564	19.184	67.712	15.267
64	1HD2	ASN	564	22.013	69.437	18.178
65	2HD2	ASN	564	20.718	70.064	19.073
66	N	MET	565	15.876	68.982	15.969
67	CA	MET	565	14.505	69.517	16.086
68	CB	MET	565	13.941	70.565	15.096
69	CG	MET	565	13.884	71.995	15.667
70	SD	MET	565	15.501	72.811	15.848
71	CE	MET	565	14.936	74.510	16.210
72	C	MET	565	13.523	68.316	16.120
73	O	MET	565	12.755	68.248	17.069
74	HN	MET	565	16.356	69.053	15.074
75	N	LEU	566	13.511	67.417	15.005
76	CA	LEU	566	12.680	66.204	14.995
77	CB	LEU	566	12.958	65.320	13.758
78	CG	LEU	566	11.899	64.218	13.505
79	CD1	LEU	566	10.472	64.760	13.312
80	CD2	LEU	566	12.276	63.386	12.274
81	C	LEU	566	12.864	65.372	16.314
82	O	LEU	566	11.991	64.589	16.666
83	HN	LEU	566	14.194	67.502	14.256
84	N	GLY	567	14.065	65.634	17.074
85	CA	GLY	567	14.368	65.122	18.410
86	C	GLY	567	13.395	65.818	19.373
87	O	GLY	567	12.470	65.164	19.815
88	HN	GLY	567	14.755	66.315	16.727
89	N	GLY	568	13.610	67.204	19.643
90	CA	GLY	568	12.543	67.993	20.319
91	C	GLY	568	11.085	67.356	20.210
92	O	GLY	568	10.571	66.926	21.229
93	HN	GLY	568	14.527	67.648	19.464
94	N	GLN	570	9.435	64.691	18.381
95	CA	GLN	570	9.047	63.293	18.600
96	CB	GLN	570	9.949	62.264	17.954
97	CG	GLN	570	9.720	61.923	16.466
98	CD	GLN	570	10.263	60.509	16.247
99	OE1	GLN	570	9.774	59.737	15.440
100	NE2	GLN	570	11.375	60.181	17.074

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101	C	GLN	570	9.122	62.923	20.112
102	O	GLN	570	8.291	62.153	20.562
103	HN	GLN	570	10.403	64.886	18.148
104	1HE2	GLN	570	11.793	59.248	17.045
105	2HE2	GLN	570	11.654	60.884	17.791
106	N	VAL	571	10.216	63.398	20.902
107	CA	VAL	571	10.426	62.911	22.293
108	CB	VAL	571	11.858	63.181	22.856
109	CG1	VAL	571	12.086	62.848	24.356
110	CG2	VAL	571	12.908	62.362	22.069
111	C	VAL	571	9.247	63.480	23.196
112	O	VAL	571	9.117	63.034	24.321
113	HN	VAL	571	10.991	63.862	20.446
114	N	TRP	600	14.536	57.459	26.142
115	CA	TRP	600	14.286	58.373	25.033
116	CB	TRP	600	14.536	59.885	25.241
117	CG	TRP	600	15.942	60.382	25.547
118	CD2	TRP	600	16.813	61.177	24.647
119	CE2	TRP	600	17.938	61.507	25.406
120	CE3	TRP	600	16.684	61.587	23.302
121	CD1	TRP	600	16.677	60.278	26.692
122	NE1	TRP	600	17.971	60.868	26.641
123	CZ2	TRP	600	18.944	62.371	24.931
124	CZ3	TRP	600	17.722	62.405	22.786
125	CH2	TRP	600	18.804	62.836	23.600
126	C	TRP	600	15.102	57.802	23.846
127	O	TRP	600	14.500	57.522	22.826
128	HN	TRP	600	14.723	57.833	27.064
129	HE1	TRP	600	18.815	60.295	26.697
130	N	MET	601	16.503	57.579	23.980
131	CA	MET	601	17.340	57.410	22.781
132	CB	MET	601	18.846	57.418	23.119
133	CG	MET	601	19.743	57.697	21.905
134	SD	MET	601	19.495	59.370	21.193
135	CE	MET	601	20.712	60.293	22.193
136	C	MET	601	16.991	56.112	21.981
137	O	MET	601	17.166	56.100	20.777
138	HN	MET	601	16.954	58.108	24.708
139	N	MET	604	13.789	56.337	20.103
140	CA	MET	604	14.221	56.912	18.813
141	CB	MET	604	15.241	58.084	18.878
142	CG	MET	604	14.883	59.305	19.753
143	SD	MET	604	13.383	60.194	19.224
144	CE	MET	604	12.124	59.378	20.277
145	C	MET	604	14.836	55.772	17.917
146	O	MET	604	14.376	55.567	16.809
147	HN	MET	604	14.289	56.598	20.957
148	N	ALA	605	16.001	55.112	18.403
149	CA	ALA	605	16.978	54.442	17.507
150	CB	ALA	605	18.203	53.924	18.267
151	C	ALA	605	16.325	53.250	16.752
152	O	ALA	605	16.626	52.982	15.592
153	HN	ALA	605	16.380	55.356	19.311
154	N	PHE	606	15.361	52.586	17.574
155	CA	PHE	606	14.666	51.352	17.214

5	156	CB	PHE	606	13.830	50.825	18.391
	157	CG	PHE	606	13.363	49.414	18.133
	158	CD1	PHE	606	14.303	48.329	18.243
	159	CD2	PHE	606	11.979	49.117	17.871
	160	CE1	PHE	606	13.894	46.982	18.032
	161	CE2	PHE	606	11.568	47.761	17.629
	162	CZ	PHE	606	12.541	46.700	17.660
	163	C	PHE	606	13.748	51.686	16.029
10	164	O	PHE	606	13.790	50.980	15.040
	165	HN	PHE	606	15.215	52.914	18.530
	166	N	ALA	607	12.903	52.830	16.191
	167	CA	ALA	607	11.863	53.392	15.284
	168	CB	ALA	607	10.919	54.387	15.994
	169	C	ALA	607	12.445	54.123	13.996
15	170	O	ALA	607	11.819	54.073	12.944
	171	HN	ALA	607	12.937	53.245	17.125
	172	N	LEU	608	13.643	54.902	14.103
	173	CA	LEU	608	14.415	55.258	12.889
	174	CB	LEU	608	15.872	55.766	13.015
20	175	CG	LEU	608	16.535	56.170	11.672
	176	CD1	LEU	608	15.564	56.947	10.783
	177	CD2	LEU	608	17.744	57.096	11.876
	178	C	LEU	608	14.527	53.974	12.051
	179	O	LEU	608	14.127	53.955	10.899
25	180	HN	LEU	608	14.169	54.816	14.968
	181	N	GLY	609	15.072	52.871	12.762
	182	CA	GLY	609	15.130	51.566	12.135
	183	C	GLY	609	13.878	51.185	11.368
	184	O	GLY	609	13.970	50.700	10.245
30	185	HN	GLY	609	15.265	52.896	13.770
	186	N	ARG	611	10.880	53.198	10.162
	187	CA	ARG	611	10.368	53.648	8.778
	188	CB	ARG	611	9.869	55.007	8.239
	189	CG	ARG	611	8.729	55.665	9.011
	190	CD	ARG	611	9.283	56.945	9.610
35	191	NE	ARG	611	10.457	56.745	10.480
	192	CZ	ARG	611	10.610	57.593	11.582
	193	NH1	ARG	611	9.812	58.685	11.785
	194	NH2	ARG	611	11.554	57.401	12.563
	195	C	ARG	611	11.487	53.314	7.767
40	196	O	ARG	611	11.211	53.119	6.594
	197	HN	ARG	611	11.128	53.875	10.893
	198	HE	ARG	611	11.063	55.964	10.255
	199	1HH1	ARG	611	9.920	59.306	12.572
	200	2HH1	ARG	611	9.092	58.880	11.120
45	201	1HH2	ARG	611	11.603	58.057	13.338
	202	2HH2	ARG	611	12.199	56.633	12.574
	203	N	LEU	621	18.327	56.358	5.645
	204	CA	LEU	621	17.892	56.466	7.047
	205	CB	LEU	621	18.922	57.150	7.968
	206	CG	LEU	621	20.091	56.281	8.447
50	207	CD1	LEU	621	20.935	57.119	9.419
	208	CD2	LEU	621	19.593	54.989	9.109
	209	C	LEU	621	16.629	57.328	6.938
	210	O	LEU	621	16.839	58.529	6.960

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211	HN	LEU	621	19.234	56.744	5.456
212	N	CYS	622	15.306	56.815	6.729
213	CA	CYS	622	14.234	57.828	6.639
214	CB	CYS	622	12.926	57.233	6.114
215	SG	CYS	622	13.160	56.480	4.471
216	C	CYS	622	14.056	58.457	8.070
217	O	CYS	622	13.430	57.849	8.930
218	HN	CYS	622	15.072	55.855	7.001
219	HG	CYS	622	13.936	55.462	4.807
220	N	PHE	623	14.654	59.748	8.325
221	CA	PHE	623	14.539	60.297	9.730
222	CB	PHE	623	15.401	61.531	10.118
223	CG	PHE	623	16.792	61.075	10.519
224	CD1	PHE	623	17.717	60.632	9.510
225	CD2	PHE	623	17.211	61.046	11.907
226	CE1	PHE	623	19.023	60.154	9.875
227	CE2	PHE	623	18.543	60.603	12.269
228	CZ	PHE	623	19.450	60.148	11.243
229	C	PHE	623	13.037	60.614	10.025
230	O	PHE	623	12.538	60.486	11.136
231	HN	PHE	623	15.054	60.333	7.580
232	N	ALA	624	12.406	61.114	8.853
233	CA	ALA	624	11.113	61.720	8.500
234	CB	ALA	624	11.040	63.230	8.800
235	C	ALA	624	11.011	61.564	6.937
236	O	ALA	624	11.997	61.723	6.236
237	HN	ALA	624	13.007	60.967	8.040
238	N	ILE	629	18.455	60.562	4.653
239	CA	ILE	629	19.897	60.753	4.531
240	CB	ILE	629	20.661	60.701	5.882
241	CG2	ILE	629	22.180	60.700	5.633
242	CG1	ILE	629	20.202	61.914	6.757
243	CD1	ILE	629	21.100	62.288	7.948
244	C	ILE	629	20.234	59.677	3.467
245	O	ILE	629	20.440	58.503	3.743
246	HN	ILE	629	18.175	59.971	5.421
247	N	CYS	638	31.034	64.418	9.081
248	CA	CYS	638	30.921	63.606	10.354
249	CB	CYS	638	30.871	64.542	11.581
250	SG	CYS	638	32.117	65.871	11.538
251	C	CYS	638	29.661	62.632	10.415
252	O	CYS	638	29.460	62.015	11.451
253	HN	CYS	638	30.213	64.921	8.792
254	HG	CYS	638	33.063	65.261	12.246
255	N	MET	639	28.777	62.501	9.293
256	CA	MET	639	27.531	61.705	9.308
257	CB	MET	639	26.619	61.890	8.061
258	CG	MET	639	25.304	62.647	8.306
259	SD	MET	639	25.528	64.439	8.562
260	CE	MET	639	23.886	64.822	9.258
261	C	MET	639	27.781	60.167	9.463
262	O	MET	639	27.214	59.637	10.405
263	HN	MET	639	28.926	63.047	8.457
264	N	GLN	642	28.314	58.322	12.657
265	CA	GLN	642	27.386	58.403	13.783

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266	CB	GLN	642	27.149	59.910	13.979
267	CG	GLN	642	28.513	60.516	14.419
268	CD	GLN	642	28.943	59.776	15.690
269	OE1	GLN	642	28.125	59.689	16.582
270	NE2	GLN	642	30.231	59.214	15.889
271	C	GLN	642	26.125	57.570	13.438
272	O	GLN	642	25.600	56.815	14.249
273	HN	GLN	642	28.450	59.189	12.137
274	1HE2	GLN	642	30.419	58.883	16.846
275	2HE2	GLN	642	30.820	59.014	15.082
276	N	CYS	643	25.630	57.792	12.127
277	CA	CYS	643	24.401	57.297	11.541
278	CB	CYS	643	24.216	58.034	10.196
279	SG	CYS	643	23.694	59.790	10.338
280	C	CYS	643	24.479	55.742	11.373
281	O	CYS	643	23.439	55.131	11.153
282	HN	CYS	643	26.203	58.317	11.470
283	HG	CYS	643	23.042	59.851	9.179
284	N	MET	646	22.352	53.505	13.602
285	CA	MET	646	20.895	53.587	13.333
286	CB	MET	646	20.467	55.015	12.990
287	CG	MET	646	20.910	56.120	13.959
288	SD	MET	646	20.663	57.723	13.144
289	CE	MET	646	21.900	58.682	14.059
290	C	MET	646	20.579	52.798	12.031
291	O	MET	646	19.508	52.233	11.852
292	HN	MET	646	22.870	54.262	13.186
293	N	VAL	729	22.065	52.181	21.522
294	CA	VAL	729	21.631	53.332	22.332
295	CB	VAL	729	20.716	52.951	23.514
296	CG1	VAL	729	20.710	53.987	24.657
297	CG2	VAL	729	19.304	52.701	22.983
298	C	VAL	729	22.872	54.072	22.877
299	O	VAL	729	22.863	55.289	22.841
300	HN	VAL	729	21.984	51.226	21.920
301	N	ASN	731	26.329	54.014	21.825
302	CA	ASN	731	27.138	54.820	20.870
303	CB	ASN	731	27.387	54.229	19.463
304	CG	ASN	731	28.845	53.776	19.317
305	OD1	ASN	731	29.653	54.382	18.627
306	ND2	ASN	731	29.150	52.557	19.959
307	C	ASN	731	26.443	56.202	20.692
308	O	ASN	731	27.108	57.230	20.731
309	HN	ASN	731	26.219	53.014	21.649
310	1HD2	ASN	731	30.063	52.119	20.012
311	2HD2	ASN	731	28.472	52.206	20.626
312	N	LEU	732	25.048	56.174	20.372
313	CA	LEU	732	24.290	57.406	20.172
314	CB	LEU	732	22.800	57.211	19.824
315	CG	LEU	732	22.433	56.300	18.630
316	CD1	LEU	732	20.909	56.239	18.525
317	CD2	LEU	732	23.040	56.667	17.267
318	C	LEU	732	24.382	58.269	21.468
319	O	LEU	732	24.564	59.463	21.309
320	HN	LEU	732	24.504	55.309	20.391

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321	N	LEU	733	24.161	57.703	22.765
322	CA	LEU	733	24.202	58.620	23.921
323	CB	LEU	733	24.049	57.968	25.301
324	CG	LEU	733	22.612	57.462	25.553
325	CD1	LEU	733	22.698	56.176	26.382
326	CD2	LEU	733	21.724	58.557	26.193
327	C	LEU	733	25.552	59.366	23.917
328	O	LEU	733	25.570	60.542	24.226
329	HN	LEU	733	24.452	56.716	22.873
330	N	ASN	734	26.726	58.640	23.601
331	CA	ASN	734	28.055	59.253	23.617
332	CB	ASN	734	29.217	58.329	23.269
333	CG	ASN	734	29.132	57.030	24.049
334	OD1	ASN	734	28.749	56.886	25.196
335	ND2	ASN	734	29.613	55.946	23.311
336	C	ASN	734	28.100	60.449	22.627
337	O	ASN	734	28.481	61.503	23.108
338	HN	ASN	734	26.659	57.646	23.351
339	1HD2	ASN	734	29.561	55.063	23.808
340	2HD2	ASN	734	29.782	55.936	22.305
341	N	TYR	735	27.804	60.285	21.227
342	CA	TYR	735	28.040	61.488	20.385
343	CB	TYR	735	27.995	61.224	18.877
344	CG	TYR	735	28.410	62.390	17.981
345	CD1	TYR	735	27.587	62.809	16.877
346	CE1	TYR	735	28.050	63.814	15.945
347	CD2	TYR	735	29.695	63.022	18.119
348	CE2	TYR	735	30.157	64.025	17.194
349	CZ	TYR	735	29.347	64.433	16.073
350	OH	TYR	735	29.775	65.405	15.187
351	C	TYR	735	27.034	62.613	20.790
352	O	TYR	735	27.369	63.784	20.800
353	HN	TYR	735	27.340	59.452	20.845
354	HH	TYR	735	30.552	65.841	15.572
355	N	CYS	736	25.709	62.223	21.091
356	CA	CYS	736	24.669	63.236	21.406
357	CB	CYS	736	23.284	62.741	21.834
358	SG	CYS	736	22.170	64.172	22.068
359	C	CYS	736	25.148	64.111	22.584
360	O	CYS	736	25.085	65.331	22.572
361	HN	CYS	736	25.569	61.233	21.285
362	HG	CYS	736	21.724	63.818	23.261
363	N	PHE	737	25.582	63.357	23.708
364	CA	PHE	737	26.089	64.021	24.917
365	CB	PHE	737	26.664	63.063	25.983
366	CG	PHE	737	25.636	62.240	26.724
367	CD1	PHE	737	24.221	62.550	26.756
368	CD2	PHE	737	26.128	61.152	27.526
369	CE1	PHE	737	23.340	61.790	27.593
370	CE2	PHE	737	25.242	60.365	28.321
371	CZ	PHE	737	23.847	60.690	28.361
372	C	PHE	737	27.229	65.005	24.499
373	O	PHE	737	27.067	66.187	24.739
374	HN	PHE	737	25.846	62.376	23.585
375	N	THR	739	28.681	66.189	21.280

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376	CA	THR	739	28.309	67.384	20.463
377	CB	THR	739	27.440	67.126	19.217
378	OG1	THR	739	26.320	66.342	19.589
379	CG2	THR	739	28.179	66.402	18.097
380	C	THR	739	27.566	68.474	21.305
381	O	THR	739	27.905	69.636	21.151
382	HN	THR	739	28.581	65.281	20.851
383	HG1	THR	739	26.729	65.628	20.104
384	N	PHE	740	26.513	68.090	22.188
385	CA	PHE	740	25.779	69.026	23.045
386	CB	PHE	740	24.652	68.371	23.870
387	CG	PHE	740	24.048	69.312	24.883
388	CD1	PHE	740	23.350	70.515	24.507
389	CD2	PHE	740	24.123	68.970	26.273
390	CE1	PHE	740	22.645	71.311	25.474
391	CE2	PHE	740	23.445	69.769	27.246
392	CZ	PHE	740	22.678	70.918	26.852
393	C	PHE	740	26.785	69.777	23.972
394	O	PHE	740	26.564	70.958	24.193
395	HN	PHE	740	26.497	67.112	22.462
396	N	ILE	747	25.929	73.116	17.326
397	CA	ILE	747	24.692	72.401	16.976
398	CB	ILE	747	24.972	70.887	16.734
399	CG2	ILE	747	23.710	70.032	16.954
400	CG1	ILE	747	25.544	70.693	15.298
401	CD1	ILE	747	26.024	69.275	14.951
402	C	ILE	747	23.693	72.719	18.146
403	O	ILE	747	24.061	72.665	19.315
404	HN	ILE	747	26.567	72.631	17.950
405	N	PHE	749	20.020	71.968	20.436
406	CA	PHE	749	19.113	70.994	21.038
407	CB	PHE	749	19.825	70.178	22.170
408	CG	PHE	749	21.123	69.551	21.674
409	CD1	PHE	749	21.249	68.133	21.434
410	CD2	PHE	749	22.271	70.378	21.389
411	CE1	PHE	749	22.491	67.570	20.946
412	CE2	PHE	749	23.466	69.834	20.808
413	CZ	PHE	749	23.576	68.425	20.575
414	C	PHE	749	17.922	71.872	21.559
415	O	PHE	749	18.158	72.657	22.462
416	HN	PHE	749	20.737	72.269	21.075
417	N	PRO	750	16.607	71.806	20.962
418	CD	PRO	750	16.137	70.841	19.982
419	CA	PRO	750	15.444	72.491	21.552
420	CB	PRO	750	14.275	72.210	20.593
421	CG	PRO	750	14.608	70.797	20.114
422	C	PRO	750	15.157	71.868	22.959
423	O	PRO	750	15.795	70.949	23.448
424	N	LEU	753	14.849	67.699	24.405
425	CA	LEU	753	16.084	66.906	24.480
426	CB	LEU	753	16.673	66.578	23.107
427	CG	LEU	753	16.010	65.374	22.410
428	CD1	LEU	753	14.477	65.428	22.363
429	CD2	LEU	753	16.598	65.289	20.994
430	C	LEU	753	17.160	67.649	25.276

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431	O	LEU	753	18.007	66.994	25.852
432	HN	LEU	753	14.524	68.016	23.508
433	N	ILE	757	18.993	65.466	27.892
434	CA	ILE	757	20.424	65.244	27.718
435	CB	ILE	757	20.977	66.101	26.557
436	CG2	ILE	757	22.499	66.188	26.626
437	CG1	ILE	757	20.534	65.490	25.217
438	CD1	ILE	757	20.687	66.440	24.033
439	C	ILE	757	21.047	65.623	29.086
440	O	ILE	757	21.490	64.780	29.839
441	HN	ILE	757	18.565	66.197	27.326
442	C1	SCH	1	17.190	58.143	15.541
443	C2	SCH	1	16.015	59.057	15.282
444	N3	SCH	1	14.994	58.476	14.773
445	O4	SCH	1	13.834	59.242	14.487
446	C5	SCH	1	13.788	60.544	14.792
447	O6	SCH	1	12.758	61.154	14.555
448	C7	SCH	1	14.949	61.278	15.410
449	C8	SCH	1	14.902	62.627	15.770
450	C9	SCH	1	16.030	63.231	16.334
451	C10	SCH	1	17.235	62.523	16.444
452	N11	SCH	1	18.388	63.110	16.871
453	1HN1	SCH	1	18.712	63.960	16.387
454	C12	SCH	1	19.107	62.649	17.866
455	C13	SCH	1	20.354	63.413	18.299
456	O14	SCH	1	20.934	64.111	17.181
457	C15	SCH	1	21.410	62.438	18.917
458	C16	SCH	1	22.124	61.455	17.927
459	C17	SCH	1	21.132	60.304	17.566
460	C18	SCH	1	23.317	60.761	18.661
461	C19	SCH	1	22.706	62.192	16.676
462	C20	SCH	1	22.302	61.853	15.372
463	C21	SCH	1	22.877	62.439	14.242
464	F22	SCH	1	22.460	62.092	13.025
465	C23	SCH	1	23.891	63.384	14.387
466	C24	SCH	1	24.279	63.770	15.670
467	C25	SCH	1	23.673	63.207	16.803
468	O26	SCH	1	24.040	63.668	18.070
469	C27	SCH	1	19.955	64.495	19.340
470	F28	SCH	1	19.524	63.898	20.483
471	F29	SCH	1	21.020	65.291	19.628
472	F30	SCH	1	18.949	65.264	18.840
473	O1	SCH	1	18.826	61.631	18.480
474	C31	SCH	1	17.249	61.161	16.108
475	C32	SCH	1	16.099	60.529	15.616
476	H14	SCH	1	21.051	65.042	17.344
477	H26	SCH	1	24.314	64.579	18.102

TABLE 7

SUBSET OF ATOMIC COORDINATES OF GR α IN COMPLEX WITH A-
222977 OBTAINED FROM MODELING OF THE CRYSTAL STRUCTURE OF
GR α IN COMPLEX WITH FP

Atom Number	Atom Name	Residue Name	Residue Number	X Coordinate	Y Coordinate	Z Coordinate
1	N	LEU	544	5.940	62.649	11.764
2	CA	LEU	544	5.974	64.102	11.777
3	CB	LEU	544	5.952	64.855	13.135
4	CG	LEU	544	6.701	64.350	14.406
5	CD1	LEU	544	6.322	65.241	15.616
6	CD2	LEU	544	6.415	62.880	14.786
7	C	LEU	544	7.164	64.437	10.826
8	O	LEU	544	8.239	63.851	10.879
9	HN	LEU	544	6.575	62.118	12.352
10	N	ALA	546	10.133	67.032	9.049
11	CA	ALA	546	11.077	67.973	9.665
12	CB	ALA	546	12.511	67.894	9.127
13	C	ALA	546	10.510	69.441	9.516
14	O	ALA	546	10.418	70.171	10.499
15	HN	ALA	546	10.336	66.691	8.101
16	N	THR	556	26.536	69.607	7.321
17	CA	THR	556	26.715	68.666	8.452
18	CB	THR	556	28.220	68.488	8.917
19	OG1	THR	556	29.146	68.162	7.870
20	CG2	THR	556	28.374	67.408	10.003
21	C	THR	556	25.830	69.166	9.633
22	O	THR	556	24.941	68.451	10.058
23	HN	THR	556	27.377	69.610	6.760
24	HG1	THR	556	30.034	68.403	8.201
25	N	ILE	559	21.645	70.029	8.828
26	CA	ILE	559	20.905	68.760	8.713
27	CB	ILE	559	21.548	67.582	7.907
28	CG2	ILE	559	20.807	66.252	8.203
29	CG1	ILE	559	21.607	67.839	6.379
30	CD1	ILE	559	22.044	66.636	5.512
31	C	ILE	559	20.752	68.306	10.169
32	O	ILE	559	19.621	68.351	10.607
33	HN	ILE	559	22.571	69.965	8.403
34	N	MET	560	21.905	67.857	10.889
35	CA	MET	560	21.941	67.369	12.260
36	CB	MET	560	23.351	67.439	12.875
37	CG	MET	560	24.324	66.388	12.320
38	SD	MET	560	26.019	66.718	12.895
39	CE	MET	560	26.828	65.234	12.229
40	C	MET	560	21.018	68.237	13.150
41	O	MET	560	20.533	67.696	14.121
42	HN	MET	560	22.823	67.966	10.473
43	N	THR	561	20.851	69.631	12.866
44	CA	THR	561	20.194	70.586	13.815
45	CB	THR	561	20.656	72.069	13.721

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46	OG1	THR	561	21.982	72.165	14.217
47	CG2	THR	561	19.786	73.052	14.525
48	C	THR	561	18.619	70.520	13.680
49	O	THR	561	17.937	70.552	14.690
50	HN	THR	561	21.449	70.022	12.137
51	HG1	THR	561	22.203	73.109	14.307
52	N	THR	562	18.041	70.553	12.371
53	CA	THR	562	16.553	70.280	12.158
54	CB	THR	562	15.755	70.434	10.825
55	OG1	THR	562	16.062	69.374	9.913
56	CG2	THR	562	15.809	71.834	10.188
57	C	THR	562	16.262	68.792	12.499
58	O	THR	562	15.144	68.430	12.862
59	HN	THR	562	18.664	70.520	11.569
60	HG1	THR	562	15.225	69.107	9.479
61	N	LEU	563	17.370	67.906	12.333
62	CA	LEU	563	17.285	66.577	12.933
63	CB	LEU	563	18.420	65.579	12.652
64	CG	LEU	563	18.147	64.632	11.465
65	CD1	LEU	563	17.912	65.376	10.149
66	CD2	LEU	563	19.291	63.626	11.351
67	C	LEU	563	17.087	66.791	14.472
68	O	LEU	563	16.099	66.310	14.993
69	HN	LEU	563	18.282	68.220	12.006
70	N	ASN	564	17.998	67.561	15.243
71	CA	ASN	564	17.762	67.781	16.699
72	CB	ASN	564	18.569	68.843	17.472
73	CG	ASN	564	20.056	68.607	17.508
74	OD1	ASN	564	20.629	67.652	17.018
75	ND2	ASN	564	20.778	69.585	18.188
76	C	ASN	564	16.319	68.294	16.953
77	O	ASN	564	15.795	68.053	18.031
78	HN	ASN	564	18.920	67.829	14.913
79	1HD2	ASN	564	21.765	69.634	17.976
80	2HD2	ASN	564	20.395	70.383	18.697
81	N	MET	565	15.684	69.107	15.971
82	CA	MET	565	14.312	69.583	16.188
83	CB	MET	565	13.648	70.584	15.211
84	CG	MET	565	13.656	72.043	15.707
85	SD	MET	565	15.315	72.785	15.771
86	CE	MET	565	14.869	74.511	16.170
87	C	MET	565	13.443	68.305	16.265
88	O	MET	565	12.678	68.164	17.205
89	HN	MET	565	16.160	69.310	15.099
90	N	LEU	566	13.547	67.404	15.171
91	CA	LEU	566	12.768	66.143	15.153
92	CB	LEU	566	12.945	65.257	13.893
93	CG	LEU	566	11.822	64.204	13.676
94	CD1	LEU	566	10.450	64.837	13.381
95	CD2	LEU	566	12.147	63.224	12.538
96	C	LEU	566	13.005	65.328	16.485
97	O	LEU	566	12.081	64.676	16.948
98	HN	LEU	566	14.426	67.455	14.649
99	N	GLY	567	14.263	65.502	17.171
100	CA	GLY	567	14.521	65.160	18.589

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101	C	GLY	567	13.465	65.833	19.538
102	O	GLY	567	12.547	65.132	19.919
103	HN	GLY	567	15.052	66.005	16.742
104	N	GLY	568	13.544	67.218	19.887
105	CA	GLY	568	12.411	67.926	20.537
106	C	GLY	568	10.982	67.303	20.254
107	O	GLY	568	10.368	66.848	21.205
108	HN	GLY	568	14.433	67.732	19.807
109	N	GLN	570	9.428	64.685	18.396
110	CA	GLN	570	9.049	63.281	18.604
111	CB	GLN	570	9.956	62.258	17.949
112	CG	GLN	570	9.753	61.961	16.450
113	CD	GLN	570	10.308	60.556	16.193
114	OE1	GLN	570	9.806	59.796	15.383
115	NE2	GLN	570	11.431	60.213	17.001
116	C	GLN	570	9.137	62.898	20.110
117	O	GLN	570	8.332	62.097	20.551
118	HN	GLN	570	10.392	64.875	18.141
119	1HE2	GLN	570	11.718	59.230	17.040
120	2HE2	GLN	570	11.633	60.875	17.778
121	N	VAL	571	10.216	63.398	20.902
122	CA	VAL	571	10.426	62.911	22.293
123	CB	VAL	571	11.858	63.181	22.856
124	CG1	VAL	571	12.086	62.848	24.356
125	CG2	VAL	571	12.908	62.362	22.069
126	C	VAL	571	9.247	63.480	23.196
127	O	VAL	571	9.117	63.034	24.321
128	HN	VAL	571	10.991	63.862	20.446
129	N	TRP	600	14.561	57.460	26.114
130	CA	TRP	600	14.324	58.379	25.003
131	CB	TRP	600	14.614	59.891	25.199
132	CG	TRP	600	16.028	60.382	25.501
133	CD2	TRP	600	16.930	61.120	24.578
134	CE2	TRP	600	18.065	61.447	25.325
135	CE3	TRP	600	16.817	61.490	23.221
136	CD1	TRP	600	16.747	60.323	26.661
137	NE1	TRP	600	18.055	60.884	26.595
138	CZ2	TRP	600	19.117	62.236	24.814
139	CZ3	TRP	600	17.893	62.235	22.669
140	CH2	TRP	600	19.012	62.627	23.455
141	C	TRP	600	15.100	57.770	23.809
142	O	TRP	600	14.466	57.424	22.825
143	HN	TRP	600	14.787	57.825	27.028
144	HE1	TRP	600	18.880	60.300	26.729
145	N	MET	601	16.514	57.610	23.896
146	CA	MET	601	17.323	57.405	22.681
147	CB	MET	601	18.834	57.412	22.988
148	CG	MET	601	19.686	57.683	21.742
149	SD	MET	601	19.546	59.415	21.169
150	CE	MET	601	20.901	60.143	22.156
151	C	MET	601	16.967	56.077	21.930
152	O	MET	601	17.102	56.001	20.724
153	HN	MET	601	16.971	58.124	24.636
154	N	LEU	603	13.772	54.432	22.178
155	CA	LEU	603	12.454	54.451	21.540

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156	CB	LEU	603	11.434	55.244	22.366
157	CG	LEU	603	11.150	54.507	23.695
158	CD1	LEU	603	10.728	55.452	24.824
159	CD2	LEU	603	10.128	53.394	23.427
160	C	LEU	603	12.673	55.106	20.169
161	O	LEU	603	12.125	54.614	19.199
162	HN	LEU	603	13.876	54.975	23.034
163	N	MET	604	13.566	56.217	20.107
164	CA	MET	604	13.981	56.821	18.842
165	CB	MET	604	14.970	58.010	18.972
166	CG	MET	604	14.581	59.213	19.859
167	SD	MET	604	13.063	60.070	19.348
168	CE	MET	604	11.823	59.245	20.415
169	C	MET	604	14.636	55.715	17.935
170	O	MET	604	14.173	55.510	16.829
171	HN	MET	604	13.925	56.631	20.966
172	N	ALA	605	15.861	55.133	18.370
173	CA	ALA	605	16.781	54.474	17.414
174	CB	ALA	605	18.140	54.054	18.003
175	C	ALA	605	16.114	53.230	16.751
176	O	ALA	605	16.374	52.946	15.589
177	HN	ALA	605	16.240	55.310	19.293
178	N	PHE	606	15.195	52.543	17.598
179	CA	PHE	606	14.513	51.298	17.216
180	CB	PHE	606	13.747	50.755	18.425
181	CG	PHE	606	13.304	49.339	18.170
182	CD1	PHE	606	14.259	48.269	18.295
183	CD2	PHE	606	11.931	49.029	17.874
184	CE1	PHE	606	13.870	46.921	18.067
185	CE2	PHE	606	11.543	47.672	17.614
186	CZ	PHE	606	12.529	46.627	17.662
187	C	PHE	606	13.506	51.591	16.073
188	O	PHE	606	13.333	50.781	15.180
189	HN	PHE	606	15.064	52.882	18.553
190	N	ALA	607	12.820	52.837	16.170
191	CA	ALA	607	11.742	53.395	15.301
192	CB	ALA	607	10.836	54.405	16.040
193	C	ALA	607	12.289	54.110	13.992
194	O	ALA	607	11.664	54.064	12.939
195	HN	ALA	607	13.125	53.441	16.939
196	N	LEU	608	13.478	54.884	14.096
197	CA	LEU	608	14.239	55.248	12.891
198	CB	LEU	608	15.611	55.891	13.143
199	CG	LEU	608	16.409	56.104	11.838
200	CD1	LEU	608	15.637	57.041	10.912
201	CD2	LEU	608	17.811	56.651	12.114
202	C	LEU	608	14.475	53.960	12.058
203	O	LEU	608	14.118	53.927	10.891
204	HN	LEU	608	14.044	54.730	14.929
205	N	GLY	609	15.072	52.871	12.762
206	CA	GLY	609	15.130	51.566	12.135
207	C	GLY	609	13.878	51.185	11.368
208	O	GLY	609	13.970	50.700	10.245
209	HN	GLY	609	15.265	52.896	13.770
210	N	ARG	611	10.857	53.193	10.139

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211	CA	ARG	611	10.355	53.632	8.752
212	CB	ARG	611	9.843	54.982	8.210
213	CG	ARG	611	8.689	55.607	8.985
214	CD	ARG	611	9.225	56.890	9.590
215	NE	ARG	611	10.412	56.723	10.461
216	CZ	ARG	611	10.551	57.579	11.562
217	NH1	ARG	611	9.672	58.613	11.781
218	NH2	ARG	611	11.542	57.447	12.517
219	C	ARG	611	11.489	53.310	7.755
220	O	ARG	611	11.221	53.115	6.580
221	HN	ARG	611	11.052	53.878	10.873
222	HE	ARG	611	11.054	55.975	10.220
223	1HH1	ARG	611	9.774	59.243	12.566
224	2HH1	ARG	611	8.902	58.754	11.149
225	1HH2	ARG	611	11.573	58.106	13.291
226	2HH2	ARG	611	12.233	56.718	12.509
227	N	LEU	621	18.340	56.346	5.666
228	CA	LEU	621	17.897	56.453	7.068
229	CB	LEU	621	18.926	57.115	8.017
230	CG	LEU	621	20.170	56.278	8.350
231	CD1	LEU	621	21.020	57.019	9.409
232	CD2	LEU	621	19.779	54.857	8.782
233	C	LEU	621	16.632	57.319	6.960
234	O	LEU	621	16.849	58.518	6.998
235	HN	LEU	621	19.245	56.741	5.477
236	N	CYS	622	15.306	56.815	6.729
237	CA	CYS	622	14.234	57.828	6.639
238	CB	CYS	622	12.926	57.233	6.114
239	SG	CYS	622	13.160	56.480	4.471
240	C	CYS	622	14.056	58.457	8.070
241	O	CYS	622	13.430	57.849	8.930
242	HN	CYS	622	15.072	55.855	7.001
243	HG	CYS	622	13.936	55.462	4.807
244	N	PHE	623	14.601	59.763	8.308
245	CA	PHE	623	14.425	60.309	9.705
246	CB	PHE	623	15.244	61.569	10.081
247	CG	PHE	623	16.556	61.042	10.590
248	CD1	PHE	623	17.579	60.635	9.669
249	CD2	PHE	623	16.726	60.787	11.999
250	CE1	PHE	623	18.761	59.986	10.164
251	CE2	PHE	623	17.921	60.170	12.497
252	CZ	PHE	623	18.933	59.751	11.571
253	C	PHE	623	12.921	60.569	10.011
254	O	PHE	623	12.429	60.437	11.124
255	HN	PHE	623	15.017	60.332	7.556
256	N	ALA	624	12.283	61.028	8.839
257	CA	ALA	624	11.034	61.723	8.528
258	CB	ALA	624	11.045	63.224	8.877
259	C	ALA	624	10.967	61.630	6.967
260	O	ALA	624	11.954	61.868	6.293
261	HN	ALA	624	12.896	60.941	8.021
262	N	LEU	627	12.747	64.097	4.793
263	CA	LEU	627	14.163	64.327	5.140
264	CB	LEU	627	14.482	65.265	6.339
265	CG	LEU	627	15.970	65.710	6.422

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266	CD1	LEU	627	16.199	66.758	7.534
267	CD2	LEU	627	16.940	64.529	6.608
268	C	LEU	627	14.760	62.885	5.331
269	O	LEU	627	14.829	62.358	6.436
270	HN	LEU	627	12.277	63.333	5.282
271	N	ILE	629	18.460	60.556	4.655
272	CA	ILE	629	19.905	60.734	4.555
273	CB	ILE	629	20.662	60.638	5.912
274	CG2	ILE	629	22.181	60.686	5.662
275	CG1	ILE	629	20.189	61.794	6.853
276	CD1	ILE	629	21.052	62.074	8.102
277	C	ILE	629	20.244	59.674	3.469
278	O	ILE	629	20.464	58.500	3.734
279	HN	ILE	629	18.154	59.992	5.437
280	N	MET	634	24.928	61.075	3.277
281	CA	MET	634	25.781	60.213	4.131
282	CB	MET	634	25.575	58.727	3.734
283	CG	MET	634	26.417	57.674	4.474
284	SD	MET	634	26.018	57.458	6.251
285	CE	MET	634	25.117	55.867	6.189
286	C	MET	634	27.288	60.594	3.951
287	O	MET	634	28.087	60.349	4.850
288	HN	MET	634	24.727	60.641	2.372
289	N	CYS	638	31.098	64.594	9.077
290	CA	CYS	638	31.055	64.015	10.454
291	CB	CYS	638	31.239	65.080	11.558
292	SG	CYS	638	32.568	66.285	11.216
293	C	CYS	638	29.709	63.226	10.664
294	O	CYS	638	29.190	63.165	11.770
295	HN	CYS	638	30.527	65.420	8.911
296	HG	CYS	638	33.011	66.409	12.463
297	N	MET	639	29.177	62.603	9.493
298	CA	MET	639	28.118	61.606	9.391
299	CB	MET	639	27.276	61.590	8.083
300	CG	MET	639	25.994	62.438	8.084
301	SD	MET	639	26.258	64.229	8.311
302	CE	MET	639	24.506	64.724	8.423
303	C	MET	639	28.818	60.222	9.463
304	O	MET	639	28.321	59.438	10.253
305	HN	MET	639	29.536	62.905	8.595
306	N	TYR	640	29.848	59.854	8.495
307	CA	TYR	640	29.739	58.468	7.927
308	CB	TYR	640	30.816	57.958	6.919
309	CG	TYR	640	30.450	56.539	6.491
310	CD1	TYR	640	29.652	56.268	5.315
311	CE1	TYR	640	29.053	54.968	5.129
312	CD2	TYR	640	30.769	55.432	7.359
313	CE2	TYR	640	30.153	54.145	7.178
314	CZ	TYR	640	29.243	53.913	6.093
315	OH	TYR	640	28.569	52.720	5.978
316	C	TYR	640	29.564	57.430	9.097
317	O	TYR	640	28.562	56.733	9.138
318	HN	TYR	640	30.292	60.563	7.909
319	HH	TYR	640	28.269	52.670	5.058
320	N	ASP	641	30.620	57.298	10.037

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321	CA	ASP	641	30.649	56.562	11.304
322	CB	ASP	641	31.628	57.260	12.263
323	CG	ASP	641	33.078	56.758	12.235
324	OD1	ASP	641	33.794	57.386	13.008
325	OD2	ASP	641	33.377	55.816	11.498
326	C	ASP	641	29.326	56.543	12.107
327	O	ASP	641	28.909	55.513	12.616
328	HN	ASP	641	31.416	57.909	9.941
329	N	GLN	642	28.792	57.830	12.393
330	CA	GLN	642	27.838	58.002	13.496
331	CB	GLN	642	27.603	59.502	13.734
332	CG	GLN	642	28.908	60.138	14.274
333	CD	GLN	642	29.236	59.505	15.630
334	OE1	GLN	642	28.374	59.494	16.485
335	NE2	GLN	642	30.522	58.980	15.921
336	C	GLN	642	26.552	57.241	13.119
337	O	GLN	642	25.935	56.582	13.949
338	HN	GLN	642	29.140	58.691	11.949
339	1HE2	GLN	642	30.718	58.815	16.912
340	2HE2	GLN	642	31.248	59.012	15.207
341	N	CYS	643	26.169	57.411	11.744
342	CA	CYS	643	25.074	56.740	11.046
343	CB	CYS	643	24.892	57.322	9.616
344	SG	CYS	643	24.484	59.105	9.519
345	C	CYS	643	25.277	55.166	10.943
346	O	CYS	643	24.394	54.575	10.340
347	HN	CYS	643	26.908	57.738	11.111
348	HG	CYS	643	24.214	59.154	8.216
349	N	LYS	644	26.392	54.438	11.500
350	CA	LYS	644	26.484	52.967	11.428
351	CB	LYS	644	27.925	52.366	11.385
352	CG	LYS	644	28.724	52.240	12.710
353	CD	LYS	644	30.263	52.025	12.578
354	CE	LYS	644	31.028	53.247	12.010
355	NZ	LYS	644	32.537	53.112	11.853
356	C	LYS	644	25.566	52.392	12.568
357	O	LYS	644	24.972	51.347	12.357
358	HN	LYS	644	27.136	54.909	12.007
359	HZ1	LYS	644	32.915	53.999	11.523
360	HZ2	LYS	644	33.013	52.905	12.724
361	HZ3	LYS	644	32.798	52.408	11.176
362	N	HIS	645	25.428	53.102	13.810
363	CA	HIS	645	24.598	52.550	14.900
364	CB	HIS	645	24.916	53.293	16.219
365	CG	HIS	645	26.374	52.978	16.418
366	CD2	HIS	645	26.819	51.696	16.836
367	ND1	HIS	645	27.439	53.703	15.978
368	CE1	HIS	645	28.488	52.840	16.035
369	NE2	HIS	645	28.175	51.559	16.562
370	C	HIS	645	23.061	52.510	14.519
371	O	HIS	645	22.320	51.794	15.168
372	HN	HIS	645	25.935	53.960	14.039
373	HE2	HIS	645	28.735	50.741	16.753
374	N	MET	646	22.577	53.278	13.414
375	CA	MET	646	21.229	53.597	12.908

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376	CB	MET	646	21.067	55.106	12.659
377	CG	MET	646	20.921	55.934	13.936
378	SD	MET	646	19.699	55.213	15.093
379	CE	MET	646	18.744	56.709	15.497
380	C	MET	646	20.954	52.953	11.515
381	O	MET	646	19.819	52.553	11.295
382	HN	MET	646	23.266	53.804	12.902
383	N	LEU	647	22.000	52.868	10.535
384	CA	LEU	647	21.770	51.903	9.439
385	CB	LEU	647	22.923	51.593	8.448
386	CG	LEU	647	23.029	52.476	7.171
387	CD1	LEU	647	24.271	52.062	6.344
388	CD2	LEU	647	21.765	52.405	6.279
389	C	LEU	647	21.445	50.582	10.169
390	O	LEU	647	20.690	49.782	9.652
391	HN	LEU	647	22.934	53.259	10.626
392	CD1	TYR	716	17.532	32.722	22.110
393	N	VAL	728	23.354	49.846	20.762
394	CA	VAL	728	23.256	50.881	19.702
395	CB	VAL	728	22.271	50.756	18.493
396	CG1	VAL	728	21.851	49.313	18.125
397	CG2	VAL	728	21.008	51.638	18.612
398	C	VAL	728	23.001	52.237	20.432
399	O	VAL	728	23.533	53.260	20.022
400	HN	VAL	728	22.601	49.222	21.012
401	N	VAL	729	22.065	52.181	21.522
402	CA	VAL	729	21.631	53.332	22.332
403	CB	VAL	729	20.716	52.951	23.514
404	CG1	VAL	729	20.710	53.987	24.657
405	CG2	VAL	729	19.304	52.701	22.983
406	C	VAL	729	22.872	54.072	22.877
407	O	VAL	729	22.863	55.289	22.841
408	HN	VAL	729	21.984	51.226	21.920
409	N	ASN	731	26.233	53.877	21.871
410	CA	ASN	731	27.126	54.475	20.877
411	CB	ASN	731	27.404	53.649	19.613
412	CG	ASN	731	28.901	53.366	19.468
413	OD1	ASN	731	29.507	53.633	18.446
414	ND2	ASN	731	29.519	52.667	20.519
415	C	ASN	731	26.551	55.844	20.464
416	O	ASN	731	27.349	56.736	20.226
417	HN	ASN	731	26.048	52.864	21.816
418	1HD2	ASN	731	30.318	52.062	20.364
419	2HD2	ASN	731	28.955	52.425	21.331
420	N	LEU	732	25.140	56.051	20.345
421	CA	LEU	732	24.539	57.365	20.106
422	CB	LEU	732	23.036	57.361	19.768
423	CG	LEU	732	22.579	56.463	18.601
424	CD1	LEU	732	21.077	56.679	18.381
425	CD2	LEU	732	23.394	56.658	17.311
426	C	LEU	732	24.681	58.243	21.385
427	O	LEU	732	25.033	59.396	21.210
428	HN	LEU	732	24.475	55.281	20.309
429	N	LEU	733	24.261	57.745	22.668
430	CA	LEU	733	24.302	58.675	23.822

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					24.099	58.051	25.213
431	CB	LEU	733		22.649	57.569	25.463
432	CG	LEU	733		22.699	56.282	26.294
433	CD1	LEU	733		21.767	58.663	26.114
434	CD2	LEU	733		25.667	59.408	23.841
435	C	LEU	733		25.694	60.583	24.149
436	O	LEU	733		24.463	56.738	22.837
437	HN	LEU	733		26.833	58.668	23.526
438	N	ASN	734		28.174	59.245	23.493
439	CA	ASN	734		29.260	58.246	23.120
440	CB	ASN	734		29.158	56.986	23.977
441	CG	ASN	734		28.751	56.880	25.119
442	OD1	ASN	734		29.648	55.880	23.295
443	ND2	ASN	734		28.234	60.472	22.527
444	C	ASN	734		28.553	61.514	23.068
445	O	ASN	734		26.738	57.686	23.252
446	HN	ASN	734		29.554	55.005	23.798
447	1HD2	ASN	734		29.844	55.853	22.299
448	2HD2	ASN	734		28.000	60.392	21.104
449	N	TYR	735		28.221	61.581	20.238
450	CA	TYR	735		28.239	61.209	18.744
451	CB	TYR	735		28.732	62.317	17.822
452	CG	TYR	735		27.956	62.829	16.719
453	CD1	TYR	735		28.534	63.787	15.799
454	CE1	TYR	735		30.072	62.805	17.969
455	CD2	TYR	735		30.634	63.779	17.082
456	CE2	TYR	735		29.889	64.260	15.953
457	CZ	TYR	735		30.467	65.122	15.045
458	OH	TYR	735		27.159	62.705	20.506
459	C	TYR	735		27.440	63.877	20.302
460	O	TYR	735		27.788	59.498	20.650
461	HN	TYR	735		31.333	65.397	15.397
462	HH	TYR	735		25.856	62.320	20.919
463	N	CYS	736		24.872	63.368	21.255
464	CA	CYS	736		23.401	62.968	21.477
465	CB	CYS	736		22.331	64.411	21.872
466	SG	CYS	736		25.370	64.119	22.524
467	C	CYS	736		25.411	65.337	22.520
468	O	CYS	736		25.703	61.369	21.255
469	HN	CYS	736		22.888	64.730	23.040
470	HG	CYS	736		25.665	63.340	23.679
471	N	PHE	737		26.128	63.994	24.917
472	CA	PHE	737		26.698	63.040	25.989
473	CB	PHE	737		25.668	62.221	26.731
474	CG	PHE	737		24.255	62.536	26.760
475	CD1	PHE	737		26.155	61.135	27.540
476	CD2	PHE	737		23.365	61.776	27.586
477	CE1	PHE	737		25.260	60.346	28.320
478	CE2	PHE	737		23.864	60.669	28.348
479	CZ	PHE	737		27.258	65.000	24.547
480	C	PHE	737		27.115	66.171	24.847
481	O	PHE	737		25.857	62.344	23.573
482	HN	PHE	737		28.592	66.234	21.279
483	N	THR	739		28.373	67.521	20.510
484	CA	THR	739		27.663	67.618	19.123
485	CB	THR	739				

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486	OG1	THR	739	26.244	67.699	19.219
487	CG2	THR	739	28.080	66.555	18.092
488	C	THR	739	27.622	68.587	21.389
489	O	THR	739	27.985	69.751	21.344
490	HN	THR	739	28.445	65.361	20.782
491	HG1	THR	739	25.917	66.790	19.295
492	N	PHE	740	26.510	68.154	22.175
493	CA	PHE	740	25.749	69.052	23.051
494	CB	PHE	740	24.650	68.360	23.884
495	CG	PHE	740	24.007	69.302	24.879
496	CD1	PHE	740	23.277	70.477	24.473
497	CD2	PHE	740	24.083	69.004	26.281
498	CE1	PHE	740	22.548	71.279	25.421
499	CE2	PHE	740	23.397	69.818	27.237
500	CZ	PHE	740	22.594	70.931	26.810
501	C	PHE	740	26.769	69.784	23.994
502	O	PHE	740	26.562	70.964	24.247
503	HN	PHE	740	26.262	67.166	22.125
504	N	ILE	747	25.923	73.096	17.350
505	CA	ILE	747	24.670	72.412	16.983
506	CB	ILE	747	24.877	70.891	16.705
507	CG2	ILE	747	23.621	70.043	16.988
508	CG1	ILE	747	25.331	70.694	15.231
509	CD1	ILE	747	25.758	69.266	14.865
510	C	ILE	747	23.678	72.718	18.153
511	O	ILE	747	24.023	72.615	19.325
512	HN	ILE	747	26.560	72.584	17.960
513	N	PHE	749	20.021	72.104	20.457
514	CA	PHE	749	19.101	71.157	21.062
515	CB	PHE	749	19.807	70.398	22.215
516	CG	PHE	749	20.760	69.403	21.580
517	CD1	PHE	749	20.217	68.150	21.142
518	CD2	PHE	749	22.150	69.683	21.298
519	CE1	PHE	749	21.043	67.158	20.511
520	CE2	PHE	749	22.991	68.682	20.687
521	CZ	PHE	749	22.449	67.399	20.329
522	C	PHE	749	17.913	72.042	21.523
523	O	PHE	749	18.113	72.930	22.338
524	HN	PHE	749	20.752	72.442	21.072
525	N	PRO	750	16.607	71.806	20.962
526	CD	PRO	750	16.137	70.841	19.982
527	CA	PRO	750	15.444	72.491	21.552
528	CB	PRO	750	14.275	72.210	20.593
529	CG	PRO	750	14.608	70.797	20.114
530	C	PRO	750	15.157	71.868	22.959
531	O	PRO	750	15.795	70.949	23.448
532	N	LEU	753	14.852	67.716	24.377
533	CA	LEU	753	16.127	66.985	24.320
534	CB	LEU	753	16.739	66.915	22.902
535	CG	LEU	753	16.942	65.478	22.381
536	CD1	LEU	753	15.611	64.700	22.396
537	CD2	LEU	753	17.562	65.504	20.966
538	C	LEU	753	17.154	67.647	25.242
539	O	LEU	753	17.936	66.959	25.870
540	HN	LEU	753	14.507	68.086	23.510

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	541	N	ILE	757	18.978	65.448	27.869
	542	CA	ILE	757	20.414	65.238	27.688
	543	CB	ILE	757	20.964	66.077	26.505
5	544	CG2	ILE	757	22.488	66.162	26.576
	545	CG1	ILE	757	20.521	65.482	25.146
	546	CD1	ILE	757	20.619	66.465	23.973
	547	C	ILE	757	21.045	65.622	29.064
	548	O	ILE	757	21.490	64.771	29.808
10	549	HN	ILE	757	18.553	66.213	27.348
	550	O	TYR	764	26.376	55.800	32.328
	551	C1	A22	1	16.117	63.392	13.900
	552	O2	A22	1	16.211	63.357	15.322
	553	C3	A22	1	16.477	62.074	15.719
15	554	C4	A22	1	17.785	61.634	16.122
	555	C5	A22	1	18.965	62.451	16.278
	556	C6	A22	1	18.958	63.859	16.090
	557	C7	A22	1	20.161	64.582	16.050
	558	C8	A22	1	21.372	63.974	16.417
20	559	N9	A22	1	22.523	64.796	16.383
	560	C10	A22	1	23.878	64.333	16.639
	561	C11	A22	1	24.507	65.152	17.787
	562	C12	A22	1	24.750	64.514	15.379
	563	C13	A22	1	23.850	62.882	17.067
25	564	C14	A22	1	22.777	62.061	17.215
	565	C15	A22	1	23.067	60.715	17.854
	566	C16	A22	1	21.427	62.597	16.761
	567	C17	A22	1	20.222	61.826	16.565
	568	C18	A22	1	20.280	60.320	16.495
30	569	C19	A22	1	20.998	59.992	15.189
	570	C20	A22	1	21.867	58.886	15.109
	571	C21	A22	1	22.765	58.715	14.027
	572	C22	A22	1	22.741	59.608	12.933
	573	C23	A22	1	21.800	60.663	12.950
35	574	O24	A22	1	21.777	61.595	11.938
	575	C25	A22	1	22.404	62.797	12.393
	576	S26	A22	1	22.404	62.411	13.015
	577	C27	A22	1	24.075	62.110	11.436
	578	C28	A22	1	24.904	60.815	14.035
40	579	O29	A22	1	20.908	59.614	16.702
	580	C30	A22	1	19.063	60.225	16.341
	581	C31	A22	1	17.888	59.348	16.192
	582	C32	A22	1	16.782	59.827	15.797
	583	C33	A22	1	15.519	61.209	15.618
45	584	H37	A22	1	15.360	65.630	15.808
					22.462		

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TABLE 8

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1	N	ILE	A	672	13.004	25.282	22.008	1.00	24.75
2	CA	ILE	A	672	14.475	25.215	22.242	1.00	25.11

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3	C	ILE	A	672	15.115	23.900	21.789	25.32
	4	O	ILE	A	672	16.189	23.926	21.195	24.67
	5	CB	ILE	A	672	14.846	25.527	23.734	25.78
10	6	CG1	ILE	A	672	14.842	27.035	23.978	25.60
	7	CG2	ILE	A	672	16.247	25.008	24.099	25.56
	8	CD1	ILE	A	672	15.312	27.404	25.360	25.81
15	9	N	PHE	A	673	14.448	22.768	22.030	25.89
	10	CA	PHE	A	673	14.980	21.446	21.635	25.86
	11	C	PHE	A	673	15.213	21.374	20.147	25.25
	12	O	PHE	A	673	16.260	20.926	19.680	24.38
20	13	CB	PHE	A	673	14.020	20.306	22.029	26.22
	14	CG	PHE	A	673	14.557	18.923	21.722	25.12
	15	CD1	PHE	A	673	15.765	18.501	22.251	25.16
25	16	CD2	PHE	A	673	13.877	18.066	20.874	25.81
	17	CE1	PHE	A	673	16.286	17.255	21.946	23.42
	18	CE2	PHE	A	673	14.403	16.809	20.567	25.08
	19	CZ	PHE	A	673	15.609	16.417	21.107	23.85
30	20	N	LEU	A	674	14.193	21.792	19.412	25.01
	21	CA	LEU	A	674	14.237	21.802	17.969	25.58
	22	C	LEU	A	674	15.199	22.801	17.357	25.10
35	23	O	LEU	A	674	15.743	22.518	16.294	26.08
	24	CB	LEU	A	674	12.833	21.974	17.391	26.05
	25	CG	LEU	A	674	12.067	20.653	17.317	26.55
	26	CD1	LEU	A	674	10.617	20.887	16.935	26.35
40	27	CD2	LEU	A	674	12.762	19.758	16.304	26.09
	28	N	ASN	A	675	15.440	23.939	18.019	24.63
	29	CA	ASN	A	675	16.356	24.964	17.484	23.19
45	30	C	ASN	A	675	17.726	24.338	17.397	21.66
	31	O	ASN	A	675	18.435	24.524	16.417	21.43
	32	CB	ASN	A	675	16.478	26.215	18.393	24.20
	33	CG	ASN	A	675	15.206	27.067	18.452	24.32
50	34	OD1	ASN	A	675	14.368	27.062	17.547	24.82
	35	ND2	ASN	A	675	15.076	27.817	19.539	24.74
	36	N	VAL	A	676	18.095	23.612	18.448	21.17
55	37	CA	VAL	A	676	19.394	22.952	18.507	20.92
	38	C	VAL	A	676	19.501	21.830	17.473	19.78
	39	O	VAL	A	676	20.421	21.827	16.646	19.99

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
40	CB	VAL	A	676	19.718	22.442	19.934	1.00	21.33
41	CG1	VAL	A	676	18.899	21.237	20.247	1.00	24.09
42	CG2	VAL	A	676	21.192	22.095	20.065	1.00	21.88
43	N	LEU	A	677	18.530	20.923	17.434	1.00	19.08
44	CA	LEU	A	677	18.601	19.848	16.453	1.00	17.91
45	C	LEU	A	677	18.768	20.427	15.068	1.00	16.96
46	O	LEU	A	677	19.640	20.008	14.347	1.00	14.94
47	CB	LEU	A	677	17.383	18.921	16.518	1.00	17.50
48	CG	LEU	A	677	17.267	18.083	17.798	1.00	16.78
49	CD1	LEU	A	677	16.355	16.934	17.541	1.00	17.01
50	CD2	LEU	A	677	18.615	17.555	18.225	1.00	17.10
51	N	GLU	A	678	17.980	21.445	14.736	1.00	19.12
52	CA	GLU	A	678	18.058	22.121	13.437	1.00	20.06
53	C	GLU	A	678	19.410	22.783	13.243	1.00	19.33
54	O	GLU	A	678	19.966	22.737	12.152	1.00	18.20
55	CB	GLU	A	678	16.972	23.188	13.317	1.00	23.33
56	CG	GLU	A	678	15.532	22.646	13.381	1.00	28.64
57	CD	GLU	A	678	14.459	23.736	13.387	1.00	32.31
58	OE1	GLU	A	678	14.811	24.943	13.374	1.00	34.41
59	OE2	GLU	A	678	13.253	23.384	13.410	1.00	34.91
60	N	ALA	A	679	19.966	23.324	14.329	1.00	19.45
61	CA	ALA	A	679	21.257	24.018	14.303	1.00	18.84
62	C	ALA	A	679	22.472	23.094	14.195	1.00	19.25
63	O	ALA	A	679	23.479	23.436	13.558	1.00	19.27
64	CB	ALA	A	679	21.388	24.919	15.517	1.00	17.67
65	N	ILE	A	680	22.395	21.914	14.802	1.00	18.82
66	CA	ILE	A	680	23.518	20.984	14.742	1.00	17.49
67	C	ILE	A	680	23.516	19.984	13.593	1.00	16.89
68	O	ILE	A	680	24.518	19.303	13.370	1.00	17.12
69	CB	ILE	A	680	23.674	20.231	16.056	1.00	17.05
70	CG1	ILE	A	680	22.393	19.467	16.391	1.00	15.55
71	CG2	ILE	A	680	24.022	21.213	17.158	1.00	16.83
72	CD1	ILE	A	680	22.558	18.575	17.552	1.00	13.80
73	N	GLU	A	681	22.415	19.922	12.847	1.00	16.79
74	CA	GLU	A	681	22.265	19.002	11.719	1.00	17.26
75	C	GLU	A	681	23.370	19.128	10.673	1.00	18.79
76	O	GLU	A	681	23.517	20.173	10.043	1.00	20.09

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	77	CB	GLU	A	681	20.902	19.227	11.094	1.00	16.72
	78	CG	GLU	A	681	20.579	18.300	9.952	1.00	18.48
	79	CD	GLU	A	681	20.473	16.823	10.348	1.00	17.51
10	80	OE1	GLU	A	681	20.659	16.502	11.524	1.00	17.58
	81	OE2	GLU	A	681	20.214	15.981	9.467	1.00	18.59
	82	N	PRO	A	682	24.145	18.044	10.437	1.00	19.02
15	83	CA	PRO	A	682	25.252	18.021	9.472	1.00	19.11
	84	C	PRO	A	682	24.912	18.475	8.057	1.00	19.76
	85	O	PRO	A	682	23.771	18.382	7.625	1.00	21.13
20	86	CB	PRO	A	682	25.681	16.546	9.493	1.00	18.30
	87	CG	PRO	A	682	25.338	16.109	10.846	1.00	17.08
	88	CD	PRO	A	682	23.969	16.704	11.019	1.00	18.22
25	89	N	GLY	A	683	25.901	18.995	7.339	1.00	20.64
	90	CA	GLY	A	683	25.665	19.422	5.972	1.00	21.67
	91	C	GLY	A	683	25.809	18.260	4.990	1.00	23.13
30	92	O	GLY	A	683	25.595	17.108	5.355	1.00	23.47
	93	N	VAL	A	684	26.190	18.567	3.748	1.00	23.58
	94	CA	VAL	A	684	26.365	17.573	2.685	1.00	22.44
35	95	C	VAL	A	684	27.725	16.934	2.811	1.00	20.64
	96	O	VAL	A	684	28.708	17.614	3.042	1.00	19.82
	97	CB	VAL	A	684	26.320	18.216	1.259	1.00	24.93
40	98	CG1	VAL	A	684	26.217	17.130	0.183	1.00	24.57
	99	CG2	VAL	A	684	25.153	19.228	1.131	1.00	24.89
	100	N	VAL	A	685	27.778	15.631	2.585	1.00	19.05
45	101	CA	VAL	A	685	29.012	14.878	2.665	1.00	17.89
	102	C	VAL	A	685	29.143	14.112	1.345	1.00	17.88
	103	O	VAL	A	685	28.238	13.367	0.969	1.00	18.33
50	104	CB	VAL	A	685	28.955	13.857	3.867	1.00	17.81
	105	CG1	VAL	A	685	30.303	13.189	4.086	1.00	15.58
	106	CG2	VAL	A	685	28.527	14.556	5.147	1.00	16.27
55	107	N	CYS	A	686	30.224	14.339	0.609	1.00	17.00
	108	CA	CYS	A	686	30.451	13.628	-0.650	1.00	17.52
	109	C	CYS	A	686	31.354	12.447	-0.327	1.00	16.97
60	110	O	CYS	A	686	32.141	12.496	0.615	1.00	17.15
	111	CB	CYS	A	686	31.101	14.534	-1.706	1.00	17.76
	112	SG	CYS	A	686	30.166	16.031	-2.147	1.00	21.38
65	113	N	ALA	A	687	31.183	11.360	-1.065	1.00	17.74

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	114	CA	ALA	A	687	31.949	10.132	-0.836	17.57
	115	C	ALA	A	687	33.277	10.161	-1.526	18.06
	116	O	ALA	A	687	34.185	9.431	-1.139	17.98
10	117	CB	ALA	A	687	31.161	8.929	-1.295	16.91
	118	N	GLY	A	688	33.370	11.023	-2.539	18.50
	119	CA	GLY	A	688	34.580	11.167	-3.326	19.16
	120	C	GLY	A	688	34.705	10.099	-4.388	19.90
15	121	O	GLY	A	688	35.802	9.730	-4.771	20.86
	122	N	HIS	A	689	33.582	9.630	-4.907	20.92
	123	CA	HIS	A	689	33.577	8.576	-5.912	22.43
20	124	C	HIS	A	689	33.923	9.063	-7.328	24.19
	125	O	HIS	A	689	33.511	10.145	-7.731	24.06
	126	CB	HIS	A	689	32.195	7.917	-5.900	22.00
	127	CG	HIS	A	689	32.046	6.775	-6.857	22.28
25	128	ND1	HIS	A	689	31.040	6.724	-7.796	22.44
	129	CD2	HIS	A	689	32.782	5.656	-7.033	22.64
	130	CE1	HIS	A	689	31.166	5.627	-8.516	23.43
30	131	NE2	HIS	A	689	32.219	4.960	-8.074	23.78
	132	N	ASP	A	690	34.719	8.296	-8.073	26.27
	133	CA	ASP	A	690	35.017	8.691	-9.447	28.86
	134	C	ASP	A	690	33.872	8.164	-10.286	30.15
35	135	O	ASP	A	690	33.701	6.952	-10.409	30.46
	136	CB	ASP	A	690	36.330	8.096	-9.963	28.93
	137	CG	ASP	A	690	36.696	8.618	-11.361	30.03
40	138	OD1	ASP	A	690	37.868	8.497	-11.764	31.23
	139	OD2	ASP	A	690	35.819	9.170	-12.061	29.72
	140	N	ASN	A	691	33.065	9.067	-10.832	32.35
	141	CA	ASN	A	691	31.933	8.660	-11.655	33.60
45	142	C	ASN	A	691	32.284	8.608	-13.136	35.13
	143	O	ASN	A	691	31.419	8.733	-13.999	36.66
	144	CB	ASN	A	691	30.725	9.562	-11.416	32.74
50	145	CG	ASN	A	691	30.079	9.313	-10.074	32.95
	146	OD1	ASN	A	691	29.187	8.474	-9.930	32.13
	147	ND2	ASN	A	691	30.547	10.024	-9.069	33.57
	148	N	ASN	A	692	33.565	8.471	-13.434	36.15
55	149	CA	ASN	A	692	33.995	8.365	-14.819	37.44
	150	C	ASN	A	692	34.425	6.913	-15.027	38.39

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	151	O	ASN	A	692	34.414	6.406	-16.139	1.00	39.10
	152	CB	ASN	A	692	35.148	9.328	-15.103	1.00	36.71
	153	N	GLN	A	693	34.757	6.241	-13.928	1.00	39.29
10	154	CA	GLN	A	693	35.200	4.849	-13.942	1.00	40.00
	155	C	GLN	A	693	33.988	3.939	-13.854	1.00	39.48
	156	O	GLN	A	693	32.997	4.298	-13.217	1.00	40.11
15	157	CB	GLN	A	693	36.131	4.577	-12.745	1.00	41.81
	158	CG	GLN	A	693	37.538	4.029	-13.110	1.00	44.34
	159	CD	GLN	A	693	38.420	5.017	-13.902	1.00	45.44
20	160	OE1	GLN	A	693	39.378	5.587	-13.363	1.00	45.95
	161	NE2	GLN	A	693	38.115	5.193	-15.186	1.00	45.47
	162	N	PRO	A	694	34.055	2.743	-14.485	1.00	38.78
25	163	CA	PRO	A	694	32.970	1.762	-14.489	1.00	36.98
	164	C	PRO	A	694	32.575	1.304	-13.109	1.00	35.56
	165	O	PRO	A	694	33.411	1.198	-12.204	1.00	35.44
30	166	CB	PRO	A	694	33.571	0.601	-15.265	1.00	37.17
	167	CG	PRO	A	694	34.432	1.271	-16.234	1.00	38.48
	168	CD	PRO	A	694	35.138	2.286	-15.375	1.00	38.88
35	169	N	ASP	A	695	31.289	1.022	-12.958	1.00	34.27
	170	CA	ASP	A	695	30.776	0.534	-11.698	1.00	32.38
	171	C	ASP	A	695	31.318	-0.868	-11.524	1.00	32.55
40	172	O	ASP	A	695	31.237	-1.707	-12.429	1.00	33.50
	173	CB	ASP	A	695	29.251	0.518	-11.694	1.00	29.77
	174	CG	ASP	A	695	28.660	1.901	-11.608	1.00	28.80
45	175	OD1	ASP	A	695	27.532	2.100	-12.089	1.00	27.09
	176	OD2	ASP	A	695	29.329	2.794	-11.057	1.00	28.72
	177	N	SER	A	696	32.025	-1.052	-10.424	1.00	31.71
50	178	CA	SER	A	696	32.577	-2.333	-10.077	1.00	30.42
	179	C	SER	A	696	32.340	-2.445	-8.577	1.00	30.15
	180	O	SER	A	696	32.275	-1.418	-7.885	1.00	30.10
55	181	CB	SER	A	696	34.064	-2.383	-10.425	1.00	30.43
	182	OG	SER	A	696	34.854	-1.589	-9.567	1.00	31.47
	183	N	PHE	A	697	32.104	-3.669	-8.099	1.00	28.48
55	184	CA	PHE	A	697	31.890	-3.933	-6.679	1.00	26.74
	185	C	PHE	A	697	32.956	-3.205	-5.846	1.00	26.76
	186	O	PHE	A	697	32.641	-2.393	-4.972	1.00	27.12
	187	CB	PHE	A	697	31.982	-5.442	-6.423	1.00	25.46

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
188	CG	PHE	A	697	31.781	-5.827	-4.989	1.00	24.31
189	CD1	PHE	A	697	30.536	-5.722	-4.398	1.00	24.48
190	CD2	PHE	A	697	32.845	-6.281	-4.220	1.00	24.78
191	CE1	PHE	A	697	30.344	-6.063	-3.071	1.00	24.65
192	CE2	PHE	A	697	32.659	-6.626	-2.886	1.00	24.77
193	CZ	PHE	A	697	31.406	-6.512	-2.315	1.00	24.30
194	N	ALA	A	698	34.219	-3.495	-6.140	1.00	25.86
195	CA	ALA	A	698	35.351	-2.911	-5.436	1.00	24.97
196	C	ALA	A	698	35.323	-1.402	-5.300	1.00	25.24
197	O	ALA	A	698	35.559	-0.852	-4.216	1.00	24.99
198	CB	ALA	A	698	36.596	-3.305	-6.131	1.00	25.52
199	N	ALA	A	699	35.029	-0.737	-6.414	1.00	25.11
200	CA	ALA	A	699	35.001	0.717	-6.490	1.00	23.76
201	C	ALA	A	699	33.873	1.281	-5.668	1.00	22.91
202	O	ALA	A	699	34.084	2.133	-4.795	1.00	22.51
203	CB	ALA	A	699	34.845	1.156	-7.943	1.00	24.31
204	N	LEU	A	700	32.682	0.770	-5.957	1.00	21.56
205	CA	LEU	A	700	31.440	1.185	-5.314	1.00	20.84
206	C	LEU	A	700	31.456	0.977	-3.793	1.00	20.77
207	O	LEU	A	700	30.891	1.765	-3.035	1.00	19.67
208	CB	LEU	A	700	30.274	0.397	-5.937	1.00	19.59
209	CG	LEU	A	700	29.249	0.984	-6.911	1.00	18.78
210	CD1	LEU	A	700	29.727	2.269	-7.529	1.00	18.69
211	CD2	LEU	A	700	28.952	-0.015	-7.957	1.00	17.10
212	N	LEU	A	701	32.103	-0.093	-3.350	1.00	20.77
213	CA	LEU	A	701	32.147	-0.367	-1.941	1.00	20.58
214	C	LEU	A	701	33.261	0.365	-1.241	1.00	20.86
215	O	LEU	A	701	33.126	0.734	-0.088	1.00	21.69
216	CB	LEU	A	701	32.099	-1.871	-1.670	1.00	19.52
217	CG	LEU	A	701	30.582	-2.050	-1.567	1.00	19.40
218	CD1	LEU	A	701	30.046	-2.911	-2.642	1.00	17.73
219	CD2	LEU	A	701	30.173	-2.510	-0.217	1.00	17.25
220	N	SER	A	702	34.356	0.615	-1.937	1.00	21.06
221	CA	SER	A	702	35.406	1.378	-1.316	1.00	20.96
222	C	SER	A	702	34.874	2.791	-1.105	1.00	20.81
223	O	SER	A	702	35.187	3.423	-0.103	1.00	20.82
224	CB	SER	A	702	36.632	1.400	-2.190	1.00	21.52

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	225	OG	SER	A	702	37.204	0.120	-2.175	1.00	23.71
	226	N	SER	A	703	34.023	3.250	-2.028	1.00	20.55
	227	CA	SER	A	703	33.443	4.585	-1.934	1.00	18.91
10	228	C	SER	A	703	32.470	4.678	-0.793	1.00	18.35
	229	O	SER	A	703	32.520	5.625	-0.025	1.00	18.89
	230	CB	SER	A	703	32.755	4.966	-3.224	1.00	18.44
15	231	OG	SER	A	703	33.748	5.182	-4.194	1.00	20.63
	232	N	LEU	A	704	31.596	3.684	-0.662	1.00	17.26
	233	CA	LEU	A	704	30.639	3.687	0.432	1.00	16.37
20	234	C	LEU	A	704	31.366	3.678	1.761	1.00	16.10
	235	O	LEU	A	704	30.925	4.340	2.696	1.00	16.81
	236	CB	LEU	A	704	29.691	2.497	0.342	1.00	15.19
25	237	CG	LEU	A	704	28.558	2.583	-0.660	1.00	14.03
	238	CD1	LEU	A	704	27.882	1.259	-0.748	1.00	12.28
	239	CD2	LEU	A	704	27.582	3.681	-0.235	1.00	14.48
30	240	N	ASN	A	705	32.495	2.961	1.829	1.00	16.70
	241	CA	ASN	A	705	33.307	2.863	3.049	1.00	16.66
	242	C	ASN	A	705	33.955	4.201	3.410	1.00	17.17
35	243	O	ASN	A	705	33.970	4.587	4.570	1.00	17.46
	244	CB	ASN	A	705	34.398	1.794	2.924	1.00	15.46
	245	CG	ASN	A	705	33.850	0.384	2.941	1.00	16.24
40	246	OD1	ASN	A	705	34.448	-0.512	2.385	1.00	16.82
	247	ND2	ASN	A	705	32.726	0.180	3.592	1.00	16.07
	248	N	GLU	A	706	34.512	4.882	2.415	1.00	17.04
45	249	CA	GLU	A	706	35.151	6.193	2.598	1.00	17.55
	250	C	GLU	A	706	34.089	7.180	3.069	1.00	16.10
	251	O	GLU	A	706	34.313	8.023	3.950	1.00	16.62
50	252	CB	GLU	A	706	35.739	6.668	1.258	1.00	18.93
	253	CG	GLU	A	706	36.394	8.029	1.282	1.00	21.19
	254	CD	GLU	A	706	37.488	8.146	2.347	1.00	23.68
55	255	OE1	GLU	A	706	37.586	9.225	2.978	1.00	25.14
	256	OE2	GLU	A	706	38.246	7.175	2.569	1.00	24.37
	257	N	LEU	A	707	32.927	7.076	2.445	1.00	15.13
60	258	CA	LEU	A	707	31.803	7.916	2.792	1.00	14.21
	259	C	LEU	A	707	31.461	7.634	4.228	1.00	14.91
	260	O	LEU	A	707	31.121	8.557	4.980	1.00	15.85
65	261	CB	LEU	A	707	30.604	7.579	1.925	1.00	12.85

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	262	CG	LEU	A	707	29.318	8.262	2.328	12.03
	263	CD1	LEU	A	707	29.537	9.745	2.280	13.09
	264	CD2	LEU	A	707	28.252	7.889	1.374	12.74
10	265	N	GLY	A	708	31.532	6.358	4.602	13.93
	266	CA	GLY	A	708	31.230	5.976	5.965	12.96
	267	C	GLY	A	708	32.213	6.620	6.917	13.13
	268	O	GLY	A	708	31.849	7.061	7.987	13.55
15	269	N	GLU	A	709	33.468	6.687	6.514	14.14
	270	CA	GLU	A	709	34.525	7.279	7.322	15.83
	271	C	GLU	A	709	34.334	8.775	7.486	16.65
20	272	O	GLU	A	709	34.628	9.317	8.563	17.59
	273	CB	GLU	A	709	35.874	7.046	6.658	16.73
	274	CG	GLU	A	709	37.051	7.547	7.446	18.68
	275	CD	GLU	A	709	37.573	6.514	8.401	21.63
25	276	OE1	GLU	A	709	36.766	5.660	8.826	23.39
	277	OE2	GLU	A	709	38.784	6.544	8.723	23.17
	278	N	ARG	A	710	33.845	9.427	6.428	16.70
30	279	CA	ARG	A	710	33.616	10.869	6.418	17.32
	280	C	ARG	A	710	32.376	11.230	7.218	17.85
	281	O	ARG	A	710	32.379	12.156	8.034	17.75
	282	CB	ARG	A	710	33.459	11.346	4.990	16.07
35	283	CG	ARG	A	710	34.659	11.098	4.137	16.18
	284	CD	ARG	A	710	34.329	11.498	2.706	16.39
	285	NE	ARG	A	710	35.512	11.535	1.850	15.28
40	286	CZ	ARG	A	710	35.587	12.246	0.733	15.30
	287	NH1	ARG	A	710	34.550	12.975	0.357	14.96
	288	NH2	ARG	A	710	36.691	12.242	0.001	14.89
	289	N	GLN	A	711	31.291	10.516	6.955	18.71
45	290	CA	GLN	A	711	30.067	10.745	7.697	19.38
	291	C	GLN	A	711	30.209	10.494	9.188	19.48
	292	O	GLN	A	711	29.564	11.183	9.985	19.57
50	293	CB	GLN	A	711	28.908	9.938	7.127	19.79
	294	CG	GLN	A	711	28.377	10.566	5.878	22.36
	295	CD	GLN	A	711	27.058	10.010	5.446	23.37
	296	OE1	GLN	A	711	26.758	9.932	4.244	25.35
55	297	NE2	GLN	A	711	26.228	9.677	6.410	24.52
	298	N	LEU	A	712	31.043	9.529	9.571	18.76

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	299	CA	LEU	A	712	31.259	9.227	10.984	1.00	19.20
	300	C	LEU	A	712	31.876	10.428	11.704	1.00	19.23
	301	O	LEU	A	712	31.507	10.743	12.834	1.00	17.65
10	302	CB	LEU	A	712	32.163	8.008	11.157	1.00	20.55
	303	CG	LEU	A	712	32.522	7.607	12.590	1.00	21.95
	304	CD1	LEU	A	712	31.288	7.641	13.484	1.00	23.43
15	305	CD2	LEU	A	712	33.132	6.223	12.586	1.00	22.57
	306	N	VAL	A	713	32.809	11.099	11.039	1.00	19.70
	307	CA	VAL	A	713	33.427	12.270	11.619	1.00	19.68
20	308	C	VAL	A	713	32.328	13.277	11.990	1.00	19.53
	309	O	VAL	A	713	32.325	13.802	13.086	1.00	20.00
	310	CB	VAL	A	713	34.453	12.859	10.658	1.00	20.01
25	311	CG1	VAL	A	713	34.722	14.292	11.001	1.00	21.16
	312	CG2	VAL	A	713	35.750	12.069	10.750	1.00	20.06
	313	N	HIS	A	714	31.330	13.434	11.128	1.00	19.20
30	314	CA	HIS	A	714	30.215	14.356	11.358	1.00	19.47
	315	C	HIS	A	714	29.183	13.885	12.383	1.00	18.83
	316	O	HIS	A	714	28.497	14.701	13.005	1.00	18.73
35	317	CB	HIS	A	714	29.498	14.658	10.038	1.00	20.77
	318	CG	HIS	A	714	30.331	15.410	9.058	1.00	21.60
	319	ND1	HIS	A	714	30.131	16.744	8.784	1.00	22.32
40	320	CD2	HIS	A	714	31.369	15.016	8.283	1.00	22.31
	321	CE1	HIS	A	714	31.005	17.139	7.876	1.00	23.41
	322	NE2	HIS	A	714	31.768	16.113	7.557	1.00	23.22
45	323	N	VAL	A	715	29.006	12.572	12.485	1.00	18.39
	324	CA	VAL	A	715	28.063	11.972	13.434	1.00	16.86
	325	C	VAL	A	715	28.667	12.166	14.817	1.00	15.60
50	326	O	VAL	A	715	27.958	12.422	15.788	1.00	15.49
	327	CB	VAL	A	715	27.869	10.435	13.134	1.00	16.78
	328	CG1	VAL	A	715	27.037	9.756	14.197	1.00	17.10
55	329	CG2	VAL	A	715	27.183	10.259	11.817	1.00	17.34
	330	N	VAL	A	716	29.986	12.077	14.913	1.00	15.13
	331	CA	VAL	A	716	30.622	12.250	16.205	1.00	15.01
60	332	C	VAL	A	716	30.419	13.681	16.708	1.00	15.83
	333	O	VAL	A	716	30.129	13.883	17.887	1.00	16.61
	334	CB	VAL	A	716	32.136	11.885	16.158	1.00	14.93
65	335	CG1	VAL	A	716	32.825	12.233	17.481	1.00	13.26

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
336	CG2	VAL	A	716	32.310	10.373	15.870	1.00	14.26
337	N	LYS	A	717	30.544	14.665	15.816	1.00	16.59
338	CA	LYS	A	717	30.390	16.082	16.183	1.00	17.20
339	C	LYS	A	717	28.951	16.387	16.534	1.00	16.77
340	O	LYS	A	717	28.658	16.931	17.593	1.00	18.49
341	CB	LYS	A	717	30.884	16.974	15.041	1.00	18.94
342	CG	LYS	A	717	32.361	16.747	14.698	1.00	22.56
343	CD	LYS	A	717	33.245	16.752	15.978	1.00	25.34
344	CE	LYS	A	717	34.294	15.609	16.007	1.00	27.06
345	NZ	LYS	A	717	34.709	15.195	17.410	1.00	27.21
346	N	TRP	A	718	28.049	15.976	15.659	1.00	15.68
347	CA	TRP	A	718	26.618	16.143	15.868	1.00	14.61
348	C	TRP	A	718	26.200	15.562	17.261	1.00	15.34
349	O	TRP	A	718	25.659	16.269	18.124	1.00	14.55
350	CB	TRP	A	718	25.889	15.442	14.689	1.00	11.97
351	CG	TRP	A	718	24.433	15.266	14.841	1.00	9.66
352	CD1	TRP	A	718	23.472	16.199	14.645	1.00	9.89
353	CD2	TRP	A	718	23.757	14.069	15.254	1.00	10.28
354	NE1	TRP	A	718	22.228	15.688	14.918	1.00	8.38
355	CE2	TRP	A	718	22.373	14.371	15.293	1.00	9.98
356	CE3	TRP	A	718	24.176	12.778	15.612	1.00	10.09
357	CZ2	TRP	A	718	21.394	13.419	15.663	1.00	9.00
358	CZ3	TRP	A	718	23.201	11.835	15.980	1.00	8.20
359	CH2	TRP	A	718	21.835	12.171	16.004	1.00	7.32
360	N	ALA	A	719	26.468	14.272	17.464	1.00	16.10
361	CA	ALA	A	719	26.143	13.559	18.683	1.00	15.03
362	C	ALA	A	719	26.623	14.346	19.881	1.00	15.62
363	O	ALA	A	719	25.857	14.646	20.785	1.00	15.85
364	CB	ALA	A	719	26.796	12.184	18.657	1.00	13.59
365	N	LYS	A	720	27.870	14.781	19.828	1.00	17.45
366	CA	LYS	A	720	28.463	15.516	20.924	1.00	18.63
367	C	LYS	A	720	27.822	16.860	21.204	1.00	18.98
368	O	LYS	A	720	27.921	17.377	22.321	1.00	19.86
369	CB	LYS	A	720	29.970	15.625	20.715	1.00	19.81
370	CG	LYS	A	720	30.644	14.292	21.012	1.00	21.18
371	CD	LYS	A	720	32.136	14.334	20.860	1.00	23.81
372	CE	LYS	A	720	32.762	12.975	21.244	1.00	25.84

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	373	NZ	LYS	A	720	32.729	12.661	22.708	1.00	26.70
	374	N	ALA	A	721	27.070	17.369	20.238	1.00	18.21
	375	CA	ALA	A	721	26.406	18.651	20.382	1.00	18.10
10	376	C	ALA	A	721	24.941	18.492	20.675	1.00	18.80
	377	O	ALA	A	721	24.192	19.485	20.660	1.00	19.16
	378	CB	ALA	A	721	26.584	19.461	19.146	1.00	17.43
15	379	N	LEU	A	722	24.518	17.247	20.904	1.00	19.00
	380	CA	LEU	A	722	23.119	16.912	21.207	1.00	19.60
	381	C	LEU	A	722	22.754	17.362	22.616	1.00	20.27
20	382	O	LEU	A	722	23.521	17.125	23.549	1.00	21.72
	383	CB	LEU	A	722	22.955	15.395	21.119	1.00	19.45
	384	CG	LEU	A	722	21.855	14.771	20.271	1.00	19.62
25	385	CD1	LEU	A	722	21.540	15.657	19.099	1.00	17.02
	386	CD2	LEU	A	722	22.298	13.382	19.815	1.00	17.38
	387	N	PRO	A	723	21.574	17.992	22.811	1.00	20.69
30	388	CA	PRO	A	723	21.211	18.428	24.167	1.00	21.24
	389	C	PRO	A	723	21.266	17.287	25.195	1.00	21.66
	390	O	PRO	A	723	20.821	16.165	24.935	1.00	21.14
35	391	CB	PRO	A	723	19.767	18.917	23.997	1.00	20.40
	392	CG	PRO	A	723	19.706	19.349	22.624	1.00	20.05
	393	CD	PRO	A	723	20.500	18.317	21.861	1.00	20.29
40	394	N	GLY	A	724	21.800	17.588	26.369	1.00	22.02
	395	CA	GLY	A	724	21.874	16.598	27.416	1.00	22.29
	396	C	GLY	A	724	22.838	15.478	27.132	1.00	23.13
45	397	O	GLY	A	724	23.076	14.658	28.004	1.00	23.78
	398	N	PHE	A	725	23.434	15.446	25.946	1.00	24.14
	399	CA	PHE	A	725	24.360	14.368	25.610	1.00	24.24
50	400	C	PHE	A	725	25.505	14.170	26.582	1.00	24.85
	401	O	PHE	A	725	25.873	13.028	26.863	1.00	23.79
	402	CB	PHE	A	725	24.915	14.554	24.214	1.00	23.59
55	403	CG	PHE	A	725	25.648	13.353	23.703	1.00	23.80
	404	CD1	PHE	A	725	24.944	12.239	23.260	1.00	22.83
	405	CD2	PHE	A	725	27.046	13.328	23.675	1.00	22.40
55	406	CE1	PHE	A	725	25.623	11.130	22.804	1.00	22.77
	407	CE2	PHE	A	725	27.731	12.226	23.221	1.00	21.05
	408	CZ	PHE	A	725	27.025	11.123	22.784	1.00	22.31
	409	N	ARG	A	726	26.083	15.270	27.070	1.00	25.97

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
410	CA	ARG	A	726	27.207	15.229	28.033	1.00	27.63
411	C	ARG	A	726	26.902	14.615	29.423	1.00	27.24
412	O	ARG	A	726	27.797	14.449	30.253	1.00	27.08
413	CB	ARG	A	726	27.831	16.620	28.204	1.00	29.27
414	CG	ARG	A	726	28.622	17.087	26.995	1.00	31.68
415	CD	ARG	A	726	29.759	16.141	26.727	1.00	34.22
416	NE	ARG	A	726	30.657	16.595	25.670	1.00	37.18
417	CZ	ARG	A	726	31.872	16.090	25.464	1.00	38.28
418	NH1	ARG	A	726	32.635	16.558	24.486	1.00	39.44
419	NH2	ARG	A	726	32.329	15.109	26.232	1.00	38.78
420	N	ASN	A	727	25.632	14.316	29.683	1.00	27.15
421	CA	ASN	A	727	25.244	13.695	30.938	1.00	26.29
422	C	ASN	A	727	25.750	12.261	30.934	1.00	26.17
423	O	ASN	A	727	25.992	11.689	31.994	1.00	27.30
424	CB	ASN	A	727	23.717	13.687	31.115	1.00	25.46
425	CG	ASN	A	727	23.118	15.085	31.195	1.00	24.95
426	OD1	ASN	A	727	21.947	15.277	30.893	1.00	24.88
427	ND2	ASN	A	727	23.909	16.055	31.628	1.00	24.54
428	N	LEU	A	728	25.895	11.673	29.749	1.00	25.64
429	CA	LEU	A	728	26.362	10.289	29.625	1.00	25.16
430	C	LEU	A	728	27.833	10.208	29.974	1.00	25.79
431	O	LEU	A	728	28.571	11.157	29.739	1.00	25.15
432	CB	LEU	A	728	26.191	9.759	28.190	1.00	22.98
433	CG	LEU	A	728	24.859	9.711	27.448	1.00	20.68
434	CD1	LEU	A	728	25.084	9.133	26.076	1.00	19.66
435	CD2	LEU	A	728	23.856	8.883	28.203	1.00	19.79
436	N	HIS	A	729	28.247	9.064	30.516	1.00	27.05
437	CA	HIS	A	729	29.642	8.808	30.871	1.00	28.68
438	C	HIS	A	729	30.450	8.772	29.577	1.00	29.25
439	O	HIS	A	729	30.003	8.182	28.594	1.00	29.28
440	CB	HIS	A	729	29.737	7.455	31.570	1.00	30.72
441	CG	HIS	A	729	31.132	7.042	31.943	1.00	33.13
442	ND1	HIS	A	729	31.460	6.603	33.209	1.00	34.21
443	CD2	HIS	A	729	32.276	6.978	31.218	1.00	33.50
444	CE1	HIS	A	729	32.744	6.293	33.247	1.00	34.64
445	NE2	HIS	A	729	33.263	6.510	32.049	1.00	34.52
446	N	VAL	A	730	31.681	9.295	29.625	1.00	30.21

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	447	CA	VAL	A	730	32.592	9.365	28.465	1.00	31.02
	448	C	VAL	A	730	32.662	8.108	27.600	1.00	30.89
	449	O	VAL	A	730	32.704	8.192	26.371	1.00	30.40
10	450	CB	VAL	A	730	34.036	9.793	28.898	1.00	32.08
	451	CG1	VAL	A	730	35.077	9.446	27.811	1.00	32.91
	452	CG2	VAL	A	730	34.074	11.284	29.176	1.00	31.86
15	453	N	ASP	A	731	32.770	6.956	28.244	1.00	30.81
	454	CA	ASP	A	731	32.819	5.709	27.509	1.00	31.55
	455	C	ASP	A	731	31.474	5.425	26.889	1.00	28.94
20	456	O	ASP	A	731	31.408	4.912	25.789	1.00	29.47
	457	CB	ASP	A	731	33.244	4.536	28.410	1.00	36.23
	458	CG	ASP	A	731	32.966	3.152	27.771	1.00	40.32
25	459	OD1	ASP	A	731	31.837	2.619	27.974	1.00	42.21
	460	OD2	ASP	A	731	33.867	2.599	27.075	1.00	42.23
	461	N	ASP	A	732	30.403	5.760	27.587	1.00	26.17
30	462	CA	ASP	A	732	29.079	5.510	27.057	1.00	24.53
	463	C	ASP	A	732	28.770	6.387	25.875	1.00	23.96
	464	O	ASP	A	732	28.030	5.982	24.981	1.00	22.56
35	465	CB	ASP	A	732	28.024	5.711	28.119	1.00	24.04
	466	CG	ASP	A	732	28.073	4.654	29.186	1.00	23.64
	467	OD1	ASP	A	732	28.728	3.592	28.984	1.00	22.31
40	468	OD2	ASP	A	732	27.444	4.904	30.231	1.00	23.89
	469	N	GLN	A	733	29.288	7.612	25.920	1.00	23.56
	470	CA	GLN	A	733	29.121	8.591	24.855	1.00	22.94
45	471	C	GLN	A	733	29.636	7.997	23.557	1.00	23.20
	472	O	GLN	A	733	28.979	8.075	22.522	1.00	23.08
	473	CB	GLN	A	733	29.942	9.847	25.166	1.00	22.73
50	474	CG	GLN	A	733	29.359	10.776	26.225	1.00	23.24
	475	CD	GLN	A	733	30.208	12.013	26.480	1.00	23.27
	476	OE1	GLN	A	733	30.018	12.696	27.477	1.00	24.33
55	477	NE2	GLN	A	733	31.130	12.316	25.577	1.00	23.47
	478	N	MET	A	734	30.853	7.459	23.625	1.00	23.37
	479	CA	MET	A	734	31.545	6.832	22.508	1.00	24.31
60	480	C	MET	A	734	30.902	5.510	22.077	1.00	23.31
	481	O	MET	A	734	30.732	5.247	20.884	1.00	23.35
	482	CB	MET	A	734	33.003	6.596	22.906	1.00	27.26
65	483	CG	MET	A	734	33.749	5.604	22.047	1.00	31.61

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
484	SD	MET	A	734	35.293	5.121	22.821	1.00	39.54
485	CE	MET	A	734	34.884	3.401	23.387	1.00	37.92
486	N	ALA	A	735	30.571	4.671	23.052	1.00	21.64
487	CA	ALA	A	735	29.939	3.390	22.788	1.00	20.44
488	C	ALA	A	735	28.644	3.570	22.013	1.00	19.23
489	O	ALA	A	735	28.398	2.905	21.015	1.00	19.59
490	CB	ALA	A	735	29.650	2.683	24.110	1.00	20.71
491	N	VAL	A	736	27.799	4.460	22.501	1.00	18.69
492	CA	VAL	A	736	26.516	4.734	21.877	1.00	17.76
493	C	VAL	A	736	26.673	5.133	20.389	1.00	18.16
494	O	VAL	A	736	25.962	4.614	19.512	1.00	17.42
495	CB	VAL	A	736	25.742	5.771	22.760	1.00	18.30
496	CG1	VAL	A	736	25.373	6.998	22.011	1.00	17.05
497	CG2	VAL	A	736	24.544	5.118	23.420	1.00	17.25
498	N	ILE	A	737	27.658	5.985	20.096	1.00	17.60
499	CA	ILE	A	737	27.914	6.429	18.724	1.00	16.31
500	C	ILE	A	737	28.352	5.216	17.904	1.00	16.74
501	O	ILE	A	737	27.853	4.982	16.812	1.00	16.09
502	CB	ILE	A	737	29.046	7.497	18.683	1.00	14.71
503	CG1	ILE	A	737	28.602	8.819	19.325	1.00	15.11
504	CG2	ILE	A	737	29.476	7.772	17.272	1.00	14.05
505	CD1	ILE	A	737	29.769	9.804	19.618	1.00	12.32
506	N	GLN	A	738	29.281	4.451	18.468	1.00	18.15
507	CA	GLN	A	738	29.850	3.260	17.845	1.00	17.97
508	C	GLN	A	738	28.904	2.111	17.548	1.00	16.76
509	O	GLN	A	738	29.249	1.226	16.788	1.00	16.47
510	CB	GLN	A	738	30.960	2.715	18.713	1.00	20.53
511	CG	GLN	A	738	32.278	3.394	18.568	1.00	23.88
512	CD	GLN	A	738	33.306	2.726	19.439	1.00	26.69
513	OE1	GLN	A	738	33.027	2.390	20.593	1.00	29.30
514	NE2	GLN	A	738	34.483	2.475	18.887	1.00	28.53
515	N	TYR	A	739	27.792	2.029	18.260	1.00	16.39
516	CA	TYR	A	739	26.819	0.983	17.995	1.00	16.41
517	C	TYR	A	739	25.721	1.527	17.100	1.00	16.45
518	O	TYR	A	739	25.138	0.793	16.295	1.00	17.63
519	CB	TYR	A	739	26.174	0.448	19.285	1.00	15.99
520	CG	TYR	A	739	27.130	-0.115	20.313	1.00	15.68

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	521	CD1	TYR	A	739	28.251	-0.852	19.950	1.00	15.41
	522	CD2	TYR	A	739	26.925	0.131	21.656	1.00	16.49
	523	CE1	TYR	A	739	29.151	-1.317	20.915	1.00	16.17
10	524	CE2	TYR	A	739	27.817	-0.321	22.624	1.00	17.09
	525	CZ	TYR	A	739	28.921	-1.040	22.253	1.00	16.83
	526	OH	TYR	A	739	29.787	-1.435	23.256	1.00	18.24
15	527	N	SER	A	740	25.453	2.822	17.195	1.00	15.61
	528	CA	SER	A	740	24.384	3.404	16.403	1.00	15.61
	529	C	SER	A	740	24.697	4.054	15.060	1.00	14.87
20	530	O	SER	A	740	23.778	4.451	14.376	1.00	15.75
	531	CB	SER	A	740	23.619	4.403	17.252	1.00	15.49
	532	OG	SER	A	740	24.512	5.421	17.682	1.00	18.39
25	533	N	TRP	A	741	25.948	4.188	14.659	1.00	14.33
	534	CA	TRP	A	741	26.202	4.835	13.382	1.00	14.83
	535	C	TRP	A	741	25.471	4.246	12.166	1.00	15.12
30	536	O	TRP	A	741	24.902	4.995	11.376	1.00	15.56
	537	CB	TRP	A	741	27.706	4.997	13.113	1.00	15.35
	538	CG	TRP	A	741	28.465	3.720	13.000	1.00	17.05
35	539	CD1	TRP	A	741	28.995	3.016	14.020	1.00	17.12
	540	CD2	TRP	A	741	28.765	2.987	11.800	1.00	17.91
	541	NE1	TRP	A	741	29.592	1.878	13.551	1.00	19.60
40	542	CE2	TRP	A	741	29.467	1.834	12.190	1.00	18.98
	543	CE3	TRP	A	741	28.505	3.193	10.434	1.00	18.66
	544	CZ2	TRP	A	741	29.915	0.876	11.266	1.00	18.79
45	545	CZ3	TRP	A	741	28.949	2.240	9.509	1.00	17.91
	546	CH2	TRP	A	741	29.644	1.098	9.934	1.00	18.35
	547	N	MET	A	742	25.391	2.920	12.034	1.00	14.55
50	548	CA	MET	A	742	24.723	2.339	10.870	1.00	12.90
	549	C	MET	A	742	23.290	2.763	10.699	1.00	12.47
	550	O	MET	A	742	22.886	3.153	9.610	1.00	13.31
55	551	CB	MET	A	742	24.785	0.815	10.866	1.00	13.16
	552	CG	MET	A	742	24.219	0.185	9.597	1.00	12.17
	553	SD	MET	A	742	25.353	0.336	8.263	1.00	15.00
55	554	CE	MET	A	742	26.462	-0.994	8.639	1.00	13.52
	555	N	GLY	A	743	22.497	2.656	11.748	1.00	12.12
	556	CA	GLY	A	743	21.102	3.057	11.663	1.00	11.81
	557	C	GLY	A	743	20.947	4.558	11.452	1.00	12.08

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
558	O	GLY	A	743	20.022	5.009	10.768	1.00	11.88
559	N	LEU	A	744	21.835	5.336	12.070	1.00	12.77
560	CA	LEU	A	744	21.817	6.797	11.972	1.00	12.22
561	C	LEU	A	744	22.087	7.258	10.563	1.00	12.20
562	O	LEU	A	744	21.424	8.173	10.080	1.00	14.22
563	CB	LEU	A	744	22.884	7.418	12.888	1.00	11.70
564	CG	LEU	A	744	22.702	7.481	14.399	1.00	9.95
565	CD1	LEU	A	744	23.967	8.075	14.954	1.00	9.77
566	CD2	LEU	A	744	21.516	8.341	14.799	1.00	9.16
567	N	MET	A	745	23.083	6.651	9.921	1.00	12.34
568	CA	MET	A	745	23.466	6.991	8.541	1.00	11.39
569	C	MET	A	745	22.462	6.498	7.508	1.00	12.29
570	O	MET	A	745	22.234	7.155	6.495	1.00	10.62
571	CB	MET	A	745	24.839	6.427	8.191	1.00	10.75
572	CG	MET	A	745	25.961	6.948	9.076	1.00	8.86
573	SD	MET	A	745	27.509	6.429	8.487	1.00	11.97
574	CE	MET	A	745	28.579	6.939	9.717	1.00	9.84
575	N	VAL	A	746	21.855	5.342	7.793	1.00	12.05
576	CA	VAL	A	746	20.874	4.733	6.934	1.00	11.50
577	C	VAL	A	746	19.605	5.565	6.942	1.00	12.13
578	O	VAL	A	746	19.000	5.792	5.907	1.00	12.72
579	CB	VAL	A	746	20.524	3.315	7.426	1.00	11.19
580	CG1	VAL	A	746	19.245	2.852	6.811	1.00	10.17
581	CG2	VAL	A	746	21.615	2.355	7.095	1.00	9.64
582	N	PHE	A	747	19.227	6.051	8.117	1.00	12.64
583	CA	PHE	A	747	18.014	6.857	8.304	1.00	12.63
584	C	PHE	A	747	18.137	8.241	7.621	1.00	13.26
585	O	PHE	A	747	17.178	8.751	7.042	1.00	13.81
586	CB	PHE	A	747	17.763	7.031	9.800	1.00	11.19
587	CG	PHE	A	747	16.411	7.542	10.126	1.00	10.00
588	CD1	PHE	A	747	15.286	6.780	9.847	1.00	9.30
589	CD2	PHE	A	747	16.253	8.798	10.700	1.00	7.79
590	CE1	PHE	A	747	14.008	7.260	10.136	1.00	8.30
591	CE2	PHE	A	747	14.996	9.293	10.993	1.00	6.75
592	CZ	PHE	A	747	13.867	8.524	10.707	1.00	8.21
593	N	ALA	A	748	19.298	8.873	7.740	1.00	12.46
594	CA	ALA	A	748	19.513	10.172	7.119	1.00	12.97

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
595	C	ALA	A	748	19.640	9.988	5.635	1.00	13.78
596	O	ALA	A	748	19.226	10.850	4.882	1.00	14.44
597	CB	ALA	A	748	20.749	10.808	7.648	1.00	11.50
598	N	MET	A	749	20.209	8.864	5.204	1.00	14.54
599	CA	MET	A	749	20.381	8.578	3.782	1.00	14.78
600	C	MET	A	749	19.023	8.390	3.142	1.00	15.85
601	O	MET	A	749	18.808	8.780	1.990	1.00	17.51
602	CB	MET	A	749	21.241	7.331	3.607	1.00	15.28
603	CG	MET	A	749	21.622	6.945	2.199	1.00	15.33
604	SD	MET	A	749	20.315	6.246	1.193	1.00	18.79
605	CE	MET	A	749	20.226	4.627	1.835	1.00	18.82
606	N	GLY	A	750	18.088	7.829	3.895	1.00	16.02
607	CA	GLY	A	750	16.748	7.618	3.384	1.00	16.34
608	C	GLY	A	750	16.057	8.956	3.225	1.00	17.79
609	O	GLY	A	750	15.263	9.135	2.289	1.00	19.00
610	N	TRP	A	751	16.361	9.897	4.121	1.00	17.36
611	CA	TRP	A	751	15.778	11.241	4.091	1.00	17.99
612	C	TRP	A	751	16.266	11.995	2.857	1.00	18.41
613	O	TRP	A	751	15.457	12.558	2.124	1.00	20.13
614	CB	TRP	A	751	16.108	12.026	5.366	1.00	16.08
615	CG	TRP	A	751	15.528	13.458	5.416	1.00	14.99
616	CD1	TRP	A	751	16.225	14.636	5.364	1.00	13.27
617	CD2	TRP	A	751	14.151	13.821	5.617	1.00	13.68
618	NE1	TRP	A	751	15.375	15.705	5.538	1.00	12.27
619	CE2	TRP	A	751	14.099	15.230	5.697	1.00	12.98
620	CE3	TRP	A	751	12.967	13.090	5.743	1.00	14.14
621	CZ2	TRP	A	751	12.907	15.926	5.899	1.00	14.74
622	CZ3	TRP	A	751	11.775	13.780	5.942	1.00	14.63
623	CH2	TRP	A	751	11.756	15.188	6.020	1.00	14.82
624	N	ARG	A	752	17.569	11.971	2.607	1.00	19.13
625	CA	ARG	A	752	18.150	12.616	1.431	1.00	19.06
626	C	ARG	A	752	17.572	12.077	0.138	1.00	20.27
627	O	ARG	A	752	17.392	12.815	-0.828	1.00	20.66
628	CB	ARG	A	752	19.644	12.380	1.389	1.00	18.53
629	CG	ARG	A	752	20.370	12.908	2.567	1.00	18.25
630	CD	ARG	A	752	21.870	12.901	2.317	1.00	17.24
631	NE	ARG	A	752	22.467	11.573	2.298	1.00	14.94

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	632	CZ	ARG	A	752	22.976	10.973	3.370	14.90
	633	NH1	ARG	A	752	22.928	11.561	4.554	14.75
	634	NH2	ARG	A	752	23.684	9.864	3.240	13.87
10	635	N	SER	A	753	17.391	10.761	0.083	22.00
	636	CA	SER	A	753	16.823	10.099	-1.093	22.25
	637	C	SER	A	753	15.434	10.635	-1.289	23.31
	638	O	SER	A	753	14.978	10.803	-2.409	23.88
15	639	CB	SER	A	753	16.716	8.590	-0.879	20.25
	640	OG	SER	A	753	17.988	8.027	-0.687	19.78
	641	N	PHE	A	754	14.762	10.870	-0.173	24.76
20	642	CA	PHE	A	754	13.405	11.375	-0.156	26.45
	643	C	PHE	A	754	13.239	12.818	-0.630	27.47
	644	O	PHE	A	754	12.543	13.100	-1.614	26.87
	645	CB	PHE	A	754	12.835	11.243	1.245	26.43
25	646	CG	PHE	A	754	11.447	11.765	1.364	28.06
	647	CD1	PHE	A	754	10.407	11.168	0.654	28.69
	648	CD2	PHE	A	754	11.184	12.895	2.118	27.96
30	649	CE1	PHE	A	754	9.126	11.703	0.687	29.47
	650	CE2	PHE	A	754	9.901	13.442	2.160	28.93
	651	CZ	PHE	A	754	8.876	12.849	1.445	29.47
	652	N	THR	A	755	13.823	13.732	0.125	29.01
35	653	CA	THR	A	755	13.725	15.134	-0.190	30.83
	654	C	THR	A	755	14.317	15.460	-1.552	32.57
	655	O	THR	A	755	13.841	16.358	-2.234	33.24
40	656	CB	THR	A	755	14.345	15.972	0.918	29.71
	657	OG1	THR	A	755	15.669	15.524	1.183	28.99
	658	CG2	THR	A	755	13.553	15.796	2.164	29.63
	659	N	ASN	A	756	15.262	14.639	-1.991	34.71
45	660	CA	ASN	A	756	15.920	14.842	-3.273	36.48
	661	C	ASN	A	756	15.360	14.065	-4.457	37.88
	662	O	ASN	A	756	14.684	14.628	-5.313	39.57
50	663	CB	ASN	A	756	17.417	14.562	-3.149	36.89
	664	CG	ASN	A	756	18.137	15.616	-2.344	37.02
	665	OD1	ASN	A	756	17.563	16.237	-1.456	39.11
	666	ND2	ASN	A	756	19.392	15.844	-2.668	37.24
55	667	N	VAL	A	757	15.654	12.773	-4.518	38.99
	668	CA	VAL	A	757	15.210	11.948	-5.633	39.74

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	669	C	VAL	A	757	13.835	11.308	-5.456	1.00	39.95
	670	O	VAL	A	757	13.501	10.335	-6.134	1.00	40.19
	671	CB	VAL	A	757	16.274	10.869	-5.971	1.00	39.96
10	672	CG1	VAL	A	757	17.639	11.540	-6.170	1.00	40.00
	673	CG2	VAL	A	757	16.354	9.819	-4.871	1.00	39.28
	674	N	ASN	A	758	13.037	11.874	-4.559	1.00	40.46
15	675	CA	ASN	A	758	11.699	11.374	-4.265	1.00	41.28
	676	C	ASN	A	758	11.622	9.858	-4.100	1.00	40.91
	677	O	ASN	A	758	10.592	9.229	-4.404	1.00	40.73
20	678	CB	ASN	A	758	10.678	11.894	-5.288	1.00	43.82
	679	CG	ASN	A	758	10.257	13.331	-5.005	1.00	44.84
	680	OD1	ASN	A	758	11.097	14.199	-4.764	1.00	46.40
25	681	ND2	ASN	A	758	8.953	13.576	-4.987	1.00	45.71
	682	N	SER	A	759	12.733	9.298	-3.612	1.00	40.04
	683	CA	SER	A	759	12.891	7.877	-3.326	1.00	38.71
30	684	C	SER	A	759	13.027	6.921	-4.532	1.00	39.24
	685	O	SER	A	759	12.833	5.711	-4.382	1.00	39.20
	686	CB	SER	A	759	11.763	7.415	-2.395	1.00	37.53
35	687	OG	SER	A	759	11.496	8.369	-1.378	1.00	34.26
	688	N	ARG	A	760	13.409	7.438	-5.704	1.00	39.12
	689	CA	ARG	A	760	13.564	6.589	-6.892	1.00	38.62
40	690	C	ARG	A	760	14.897	5.840	-6.876	1.00	36.88
	691	O	ARG	A	760	15.024	4.741	-7.426	1.00	37.48
	692	CB	ARG	A	760	13.451	7.422	-8.171	1.00	40.63
45	693	CG	ARG	A	760	13.598	6.577	-9.444	1.00	44.41
	694	CD	ARG	A	760	13.903	7.394	-10.715	1.00	46.97
	695	NE	ARG	A	760	14.534	6.544	-11.729	1.00	48.86
50	696	CZ	ARG	A	760	13.875	5.797	-12.614	1.00	49.74
	697	NH1	ARG	A	760	12.542	5.795	-12.649	1.00	50.04
	698	NH2	ARG	A	760	14.553	4.969	-13.398	1.00	49.46
55	699	N	MET	A	761	15.902	6.466	-6.275	1.00	34.87
	700	CA	MET	A	761	17.238	5.890	-6.159	1.00	32.21
	701	C	MET	A	761	17.738	6.242	-4.751	1.00	29.46
	702	O	MET	A	761	17.144	7.080	-4.075	1.00	28.57
	703	CB	MET	A	761	18.171	6.510	-7.194	1.00	33.77
	704	CG	MET	A	761	17.588	6.682	-8.571	1.00	36.10
	705	SD	MET	A	761	18.859	7.115	-9.788	1.00	40.36

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	706	CE	MET	A	761	18.737	8.904	-9.809	1.00	38.10
	707	N	LEU	A	762	18.837	5.635	-4.319	1.00	26.78
	708	CA	LEU	A	762	19.382	5.905	-2.992	1.00	24.13
10	709	C	LEU	A	762	20.458	6.968	-3.040	1.00	23.01
	710	O	LEU	A	762	21.537	6.726	-3.548	1.00	22.65
	711	CB	LEU	A	762	19.956	4.637	-2.393	1.00	24.05
15	712	CG	LEU	A	762	18.957	3.502	-2.272	1.00	23.69
	713	CD1	LEU	A	762	19.615	2.272	-1.632	1.00	23.99
	714	CD2	LEU	A	762	17.788	4.011	-1.439	1.00	24.34
20	715	N	TYR	A	763	20.162	8.132	-2.475	1.00	22.03
	716	CA	TYR	A	763	21.066	9.273	-2.450	1.00	20.69
	717	C	TYR	A	763	22.068	9.173	-1.323	1.00	18.78
25	718	O	TYR	A	763	21.910	9.828	-0.304	1.00	17.73
	719	CB	TYR	A	763	20.250	10.540	-2.266	1.00	23.12
	720	CG	TYR	A	763	20.946	11.782	-2.730	1.00	25.58
30	721	CD1	TYR	A	763	20.841	12.187	-4.052	1.00	26.87
	722	CD2	TYR	A	763	21.662	12.590	-1.841	1.00	26.77
	723	CE1	TYR	A	763	21.416	13.373	-4.492	1.00	28.03
35	724	CE2	TYR	A	763	22.247	13.789	-2.272	1.00	28.35
	725	CZ	TYR	A	763	22.107	14.172	-3.604	1.00	28.85
	726	OH	TYR	A	763	22.595	15.379	-4.047	1.00	30.59
40	727	N	PHE	A	764	23.128	8.401	-1.538	1.00	17.33
	728	CA	PHE	A	764	24.152	8.191	-0.533	1.00	16.94
	729	C	PHE	A	764	24.964	9.441	-0.375	1.00	17.39
45	730	O	PHE	A	764	25.379	9.797	0.734	1.00	17.28
	731	CB	PHE	A	764	25.086	7.078	-0.956	1.00	15.91
	732	CG	PHE	A	764	24.505	5.724	-0.807	1.00	16.79
50	733	CD1	PHE	A	764	24.211	4.961	-1.908	1.00	16.06
	734	CD2	PHE	A	764	24.267	5.205	0.450	1.00	16.83
	735	CE1	PHE	A	764	23.691	3.692	-1.756	1.00	18.06
55	736	CE2	PHE	A	764	23.748	3.941	0.606	1.00	18.27
	737	CZ	PHE	A	764	23.458	3.176	-0.496	1.00	17.80
	738	N	ALA	A	765	25.224	10.084	-1.503	1.00	17.00
55	739	CA	ALA	A	765	26.013	11.292	-1.525	1.00	16.32
	740	C	ALA	A	765	25.674	11.913	-2.841	1.00	16.66
	741	O	ALA	A	765	25.051	11.267	-3.675	1.00	16.71
	742	CB	ALA	A	765	27.479	10.957	-1.460	1.00	16.17

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	743	N	PRO	A	766	26.016	13.196	-3.032	1.00	17.18
	744	CA	PRO	A	766	25.703	13.846	-4.311	1.00	17.49
	745	C	PRO	A	766	26.429	13.161	-5.481	1.00	17.65
10	746	O	PRO	A	766	25.923	13.099	-6.598	1.00	17.73
	747	CB	PRO	A	766	26.183	15.277	-4.077	1.00	17.30
	748	CG	PRO	A	766	26.002	15.451	-2.608	1.00	17.07
15	749	CD	PRO	A	766	26.544	14.169	-2.064	1.00	15.41
	750	N	ASP	A	767	27.578	12.569	-5.166	1.00	18.27
	751	CA	ASP	A	767	28.416	11.850	-6.115	1.00	18.49
20	752	C	ASP	A	767	28.330	10.317	-5.981	1.00	17.79
	753	O	ASP	A	767	29.191	9.594	-6.476	1.00	18.69
	754	CB	ASP	A	767	29.877	12.312	-5.955	1.00	18.71
25	755	CG	ASP	A	767	30.413	12.135	-4.525	1.00	19.47
	756	OD1	ASP	A	767	29.611	12.038	-3.569	1.00	20.31
	757	OD2	ASP	A	767	31.650	12.102	-4.348	1.00	19.04
30	758	N	LEU	A	768	27.334	9.820	-5.267	1.00	18.04
	759	CA	LEU	A	768	27.164	8.379	-5.110	1.00	18.20
	760	C	LEU	A	768	25.690	8.129	-4.930	1.00	18.58
35	761	O	LEU	A	768	25.184	8.068	-3.812	1.00	17.79
	762	CB	LEU	A	768	27.955	7.809	-3.914	1.00	17.47
	763	CG	LEU	A	768	28.032	6.263	-3.786	1.00	16.12
40	764	CD1	LEU	A	768	28.641	5.671	-5.047	1.00	14.30
	765	CD2	LEU	A	768	28.850	5.846	-2.563	1.00	15.17
	766	N	VAL	A	769	24.979	8.156	-6.048	1.00	19.79
45	767	CA	VAL	A	769	23.553	7.895	-6.035	1.00	20.42
	768	C	VAL	A	769	23.373	6.609	-6.852	1.00	20.73
	769	O	VAL	A	769	23.873	6.467	-7.961	1.00	22.43
50	770	CB	VAL	A	769	22.709	9.142	-6.447	1.00	19.95
	771	CG1	VAL	A	769	23.571	10.190	-7.096	1.00	20.70
	772	CG2	VAL	A	769	21.537	8.757	-7.277	1.00	19.19
55	773	N	PHE	A	770	22.871	5.604	-6.157	1.00	19.70
	774	CA	PHE	A	770	22.683	4.277	-6.681	1.00	19.29
	775	C	PHE	A	770	21.425	4.134	-7.473	1.00	19.41
	776	O	PHE	A	770	20.367	4.583	-7.054	1.00	19.74
	777	CB	PHE	A	770	22.596	3.263	-5.503	1.00	18.44
	778	CG	PHE	A	770	23.930	2.757	-4.996	1.00	16.41
	779	CD1	PHE	A	770	25.079	3.546	-5.053	1.00	14.52

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
780	CD2	PHE	A	770	24.025	1.468	-4.459	1.00	14.96
781	CE1	PHE	A	770	26.291	3.070	-4.588	1.00	13.39
782	CE2	PHE	A	770	25.243	0.979	-3.983	1.00	13.90
783	CZ	PHE	A	770	26.383	1.786	-4.050	1.00	13.96
784	N	ASN	A	771	21.534	3.474	-8.611	1.00	20.33
785	CA	ASN	A	771	20.363	3.157	-9.410	1.00	20.23
786	C	ASN	A	771	20.278	1.636	-9.292	1.00	21.01
787	O	ASN	A	771	21.129	1.013	-8.648	1.00	20.52
788	CB	ASN	A	771	20.524	3.593	-10.864	1.00	19.33
789	CG	ASN	A	771	21.883	3.304	-11.403	1.00	18.89
790	OD1	ASN	A	771	22.574	2.408	-10.942	1.00	19.51
791	ND2	ASN	A	771	22.289	4.069	-12.382	1.00	19.02
792	N	GLU	A	772	19.258	1.043	-9.898	1.00	22.23
793	CA	GLU	A	772	19.056	-0.393	-9.841	1.00	22.51
794	C	GLU	A	772	20.282	-1.102	-10.303	1.00	22.96
795	O	GLU	A	772	20.631	-2.148	-9.785	1.00	23.89
796	CB	GLU	A	772	17.888	-0.799	-10.711	1.00	23.17
797	CG	GLU	A	772	16.562	-0.455	-10.099	1.00	24.81
798	CD	GLU	A	772	15.761	-1.672	-9.724	1.00	25.41
799	OE1	GLU	A	772	14.624	-1.488	-9.252	1.00	25.33
800	OE2	GLU	A	772	16.265	-2.803	-9.913	1.00	26.23
801	N	TYR	A	773	20.961	-0.531	-11.276	1.00	22.51
802	CA	TYR	A	773	22.158	-1.164	-11.748	1.00	22.55
803	C	TYR	A	773	23.254	-1.167	-10.680	1.00	23.17
804	O	TYR	A	773	23.969	-2.170	-10.523	1.00	24.08
805	CB	TYR	A	773	22.640	-0.492	-13.018	1.00	22.84
806	CG	TYR	A	773	23.825	-1.191	-13.593	1.00	22.80
807	CD1	TYR	A	773	23.680	-2.384	-14.304	1.00	23.02
808	CD2	TYR	A	773	25.095	-0.671	-13.418	1.00	22.59
809	CE1	TYR	A	773	24.791	-3.041	-14.837	1.00	23.77
810	CE2	TYR	A	773	26.198	-1.309	-13.938	1.00	24.43
811	CZ	TYR	A	773	26.047	-2.491	-14.643	1.00	24.22
812	OH	TYR	A	773	27.172	-3.094	-15.155	1.00	25.98
813	N	ARG	A	774	23.432	-0.044	-9.982	1.00	22.85
814	CA	ARG	A	774	24.427	0.047	-8.922	1.00	21.74
815	C	ARG	A	774	23.976	-0.796	-7.743	1.00	21.36
816	O	ARG	A	774	24.791	-1.386	-7.052	1.00	20.25

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	817	CB	ARG	A	774	24.623	1.487	-8.494	1.00	22.23
	818	CG	ARG	A	774	26.026	1.952	-8.735	1.00	22.58
	819	CD	ARG	A	774	26.073	3.066	-9.756	1.00	23.92
10	820	NE	ARG	A	774	26.048	4.383	-9.146	1.00	24.69
	821	CZ	ARG	A	774	26.961	5.328	-9.365	1.00	25.97
	822	NH1	ARG	A	774	27.982	5.111	-10.171	1.00	25.01
	823	NH2	ARG	A	774	26.837	6.509	-8.783	1.00	26.70
15	824	N	MET	A	775	22.669	-0.854	-7.512	1.00	21.93
	825	CA	MET	A	775	22.136	-1.681	-6.439	1.00	23.85
	826	C	MET	A	775	22.550	-3.136	-6.666	1.00	25.38
20	827	O	MET	A	775	22.897	-3.832	-5.733	1.00	25.75
	828	CB	MET	A	775	20.614	-1.582	-6.380	1.00	23.42
	829	CG	MET	A	775	20.121	-0.241	-5.955	1.00	23.46
25	830	SD	MET	A	775	18.333	-0.199	-5.865	1.00	26.50
	831	CE	MET	A	775	17.909	1.086	-7.064	1.00	27.26
	832	N	HIS	A	776	22.507	-3.593	-7.912	1.00	27.39
30	833	CA	HIS	A	776	22.891	-4.954	-8.262	1.00	28.41
	834	C	HIS	A	776	24.403	-5.065	-8.178	1.00	29.55
	835	O	HIS	A	776	24.923	-5.865	-7.414	1.00	30.12
35	836	CB	HIS	A	776	22.418	-5.302	-9.684	1.00	29.01
	837	CG	HIS	A	776	22.639	-6.738	-10.067	1.00	30.57
	838	ND1	HIS	A	776	23.764	-7.168	-10.739	1.00	30.81
40	839	CD2	HIS	A	776	21.877	-7.843	-9.864	1.00	30.73
	840	CE1	HIS	A	776	23.685	-8.475	-10.932	1.00	29.87
	841	NE2	HIS	A	776	22.551	-8.907	-10.411	1.00	29.53
45	842	N	LYS	A	777	25.109	-4.283	-8.989	1.00	31.13
	843	CA	LYS	A	777	26.570	-4.290	-8.980	1.00	32.73
	844	C	LYS	A	777	27.032	-3.655	-7.660	1.00	34.07
50	845	O	LYS	A	777	27.382	-2.478	-7.611	1.00	36.43
	846	CB	LYS	A	777	27.130	-3.481	-10.161	1.00	31.29
	847	CG	LYS	A	777	26.678	-3.948	-11.525	1.00	30.55
55	848	CD	LYS	A	777	27.443	-5.163	-12.003	1.00	29.83
	849	CE	LYS	A	777	28.928	-4.856	-12.116	1.00	30.35
	850	NZ	LYS	A	777	29.631	-5.860	-12.983	1.00	30.53
55	851	N	SER	A	778	26.995	-4.437	-6.596	1.00	33.74
	852	CA	SER	A	778	27.387	-4.013	-5.250	1.00	33.75
	853	C	SER	A	778	27.065	-5.204	-4.366	1.00	32.95

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	854	O	SER	A	778	27.447	-5.260	-3.194	1.00	31.80
	855	CB	SER	A	778	26.593	-2.789	-4.769	1.00	33.69
	856	OG	SER	A	778	25.254	-3.122	-4.452	1.00	33.41
10	857	N	ARG	A	779	26.344	-6.149	-4.974	1.00	32.09
	858	CA	ARG	A	779	25.926	-7.386	-4.347	1.00	31.15
	859	C	ARG	A	779	25.128	-7.063	-3.084	1.00	30.75
15	860	O	ARG	A	779	25.027	-7.880	-2.163	1.00	31.03
	861	CB	ARG	A	779	27.161	-8.256	-4.071	1.00	30.74
	862	CG	ARG	A	779	28.065	-8.415	-5.299	1.00	28.19
20	863	CD	ARG	A	779	29.338	-9.182	-4.997	1.00	26.90
	864	NE	ARG	A	779	30.284	-9.129	-6.117	1.00	26.55
	865	CZ	ARG	A	779	31.583	-9.401	-6.014	1.00	26.64
25	866	NH1	ARG	A	779	32.091	-9.753	-4.846	1.00	27.87
	867	NH2	ARG	A	779	32.398	-9.234	-7.050	1.00	26.64
	868	N	MET	A	780	24.521	-5.875	-3.097	1.00	29.82
30	869	CA	MET	A	780	23.721	-5.381	-1.990	1.00	29.36
	870	C	MET	A	780	22.262	-5.165	-2.331	1.00	29.21
	871	O	MET	A	780	21.542	-4.505	-1.566	1.00	29.43
35	872	CB	MET	A	780	24.295	-4.068	-1.473	1.00	30.17
	873	CG	MET	A	780	25.194	-4.191	-0.277	1.00	30.12
	874	SD	MET	A	780	25.835	-2.592	0.168	1.00	31.24
40	875	CE	MET	A	780	24.525	-1.995	1.114	1.00	31.13
	876	N	TYR	A	781	21.831	-5.638	-3.497	1.00	28.58
	877	CA	TYR	A	781	20.433	-5.498	-3.897	1.00	28.82
45	878	C	TYR	A	781	19.701	-6.393	-2.929	1.00	30.06
	879	O	TYR	A	781	19.984	-7.589	-2.856	1.00	32.08
	880	CB	TYR	A	781	20.229	-5.985	-5.338	1.00	27.73
50	881	CG	TYR	A	781	18.896	-5.604	-5.964	1.00	26.05
	882	CD1	TYR	A	781	18.847	-4.861	-7.140	1.00	25.95
	883	CD2	TYR	A	781	17.686	-5.984	-5.382	1.00	25.08
55	884	CE1	TYR	A	781	17.624	-4.510	-7.718	1.00	25.58
	885	CE2	TYR	A	781	16.471	-5.643	-5.955	1.00	24.57
	886	CZ	TYR	A	781	16.446	-4.904	-7.115	1.00	24.77
	887	OH	TYR	A	781	15.238	-4.572	-7.668	1.00	24.60
	888	N	SER	A	782	18.730	-5.821	-2.235	1.00	30.74
	889	CA	SER	A	782	17.935	-6.500	-1.198	1.00	31.41
	890	C	SER	A	782	18.027	-5.483	-0.070	1.00	30.50

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	891	O	SER	A	782	17.044	-4.807	0.230	1.00	30.31
	892	CB	SER	A	782	18.551	-7.836	-0.726	1.00	32.82
	893	OG	SER	A	782	17.785	-8.438	0.308	1.00	35.91
10	894	N	GLN	A	783	19.242	-5.287	0.459	1.00	29.34
	895	CA	GLN	A	783	19.455	-4.314	1.522	1.00	28.01
	896	C	GLN	A	783	19.089	-2.963	0.935	1.00	26.36
15	897	O	GLN	A	783	18.342	-2.211	1.544	1.00	26.08
	898	CB	GLN	A	783	20.900	-4.309	2.020	1.00	28.50
	899	CG	GLN	A	783	21.327	-5.532	2.805	1.00	29.62
20	900	CD	GLN	A	783	21.790	-6.634	1.900	1.00	32.01
	901	OE1	GLN	A	783	21.486	-6.621	0.714	1.00	33.24
	902	NE2	GLN	A	783	22.547	-7.587	2.436	1.00	32.18
25	903	N	CYS	A	784	19.538	-2.698	-0.290	1.00	25.49
	904	CA	CYS	A	784	19.212	-1.439	-0.956	1.00	24.45
	905	C	CYS	A	784	17.698	-1.290	-1.146	1.00	25.03
30	906	O	CYS	A	784	17.155	-0.183	-1.044	1.00	25.67
	907	CB	CYS	A	784	19.951	-1.312	-2.294	1.00	22.82
	908	SG	CYS	A	784	21.746	-0.989	-2.120	1.00	18.24
35	909	N	VAL	A	785	17.003	-2.406	-1.360	1.00	25.25
	910	CA	VAL	A	785	15.538	-2.399	-1.547	1.00	25.02
	911	C	VAL	A	785	14.864	-1.979	-0.257	1.00	23.91
40	912	O	VAL	A	785	13.881	-1.259	-0.260	1.00	24.19
	913	CB	VAL	A	785	14.987	-3.826	-1.903	1.00	25.94
	914	CG1	VAL	A	785	13.457	-3.901	-1.710	1.00	26.21
45	915	CG2	VAL	A	785	15.349	-4.195	-3.324	1.00	26.31
	916	N	ARG	A	786	15.402	-2.455	0.853	1.00	25.02
	917	CA	ARG	A	786	14.855	-2.158	2.165	1.00	25.39
50	918	C	ARG	A	786	15.083	-0.679	2.520	1.00	24.71
	919	O	ARG	A	786	14.180	-0.001	3.030	1.00	25.52
	920	CB	ARG	A	786	15.468	-3.114	3.198	1.00	26.15
55	921	CG	ARG	A	786	15.392	-4.591	2.748	1.00	28.30
	922	CD	ARG	A	786	15.314	-5.583	3.900	1.00	29.76
	923	NE	ARG	A	786	14.269	-5.206	4.851	1.00	32.39
55	924	CZ	ARG	A	786	14.292	-5.475	6.157	1.00	32.41
	925	NH1	ARG	A	786	15.301	-6.153	6.701	1.00	32.09
	926	NH2	ARG	A	786	13.326	-5.001	6.932	1.00	33.31
	927	N	MET	A	787	16.246	-0.146	2.160	1.00	23.53

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	928	CA	MET	A	787	16.548	1.252	2.463	22.11
	929	C	MET	A	787	15.736	2.173	1.588	23.39
	930	O	MET	A	787	15.387	3.281	1.997	24.11
10	931	CB	MET	A	787	18.018	1.528	2.261	20.46
	932	CG	MET	A	787	18.883	0.925	3.314	17.04
	933	SD	MET	A	787	20.578	0.861	2.788	20.46
	934	CE	MET	A	787	21.285	1.969	3.729	20.07
15	935	N	ARG	A	788	15.521	1.752	0.348	24.89
	936	CA	ARG	A	788	14.738	2.499	-0.625	26.29
	937	C	ARG	A	788	13.312	2.475	-0.090	26.13
20	938	O	ARG	A	788	12.596	3.473	-0.146	26.50
	939	CB	ARG	A	788	14.833	1.790	-1.980	28.55
	940	CG	ARG	A	788	14.166	2.474	-3.174	32.52
25	941	CD	ARG	A	788	14.217	1.541	-4.395	35.44
	942	NE	ARG	A	788	13.426	1.996	-5.540	39.11
	943	CZ	ARG	A	788	13.899	2.177	-6.783	41.32
	944	NH1	ARG	A	788	15.182	1.960	-7.081	41.94
30	945	NH2	ARG	A	788	13.079	2.567	-7.754	41.48
	946	N	HIS	A	789	12.920	1.339	0.483	26.36
	947	CA	HIS	A	789	11.587	1.173	1.052	26.76
35	948	C	HIS	A	789	11.369	2.133	2.231	26.08
	949	O	HIS	A	789	10.275	2.671	2.394	25.72
	950	CB	HIS	A	789	11.377	-0.287	1.479	29.07
	951	CG	HIS	A	789	9.970	-0.609	1.879	30.42
40	952	ND1	HIS	A	789	9.538	-0.567	3.188	32.05
	953	CD2	HIS	A	789	8.890	-0.944	1.137	31.35
	954	CE1	HIS	A	789	8.249	-0.856	3.235	32.56
45	955	NE2	HIS	A	789	7.831	-1.087	2.001	32.55
	956	N	LEU	A	790	12.413	2.318	3.048	25.92
	957	CA	LEU	A	790	12.433	3.234	4.218	25.41
	958	C	LEU	A	790	12.218	4.654	3.720	25.47
50	959	O	LEU	A	790	11.359	5.380	4.216	25.06
	960	CB	LEU	A	790	13.811	3.216	4.887	23.94
	961	CG	LEU	A	790	14.039	3.400	6.383	23.32
55	962	CD1	LEU	A	790	15.444	3.930	6.570	22.41
	963	CD2	LEU	A	790	13.047	4.324	7.014	23.17
	964	N	SER	A	791	13.040	5.056	2.757	25.60

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	965	CA	SER	A	791	12.942	6.375	2.177	1.00	26.51
	966	C	SER	A	791	11.521	6.561	1.716	1.00	26.02
	967	O	SER	A	791	10.950	7.632	1.885	1.00	26.00
10	968	CB	SER	A	791	13.851	6.446	0.973	1.00	28.35
	969	OG	SER	A	791	14.936	5.559	1.179	1.00	32.32
	970	N	GLN	A	792	10.964	5.505	1.122	1.00	26.31
15	971	CA	GLN	A	792	9.600	5.526	0.610	1.00	26.32
	972	C	GLN	A	792	8.629	5.836	1.721	1.00	24.88
	973	O	GLN	A	792	7.702	6.610	1.528	1.00	24.96
20	974	CB	GLN	A	792	9.237	4.200	-0.112	1.00	28.65
	975	CG	GLN	A	792	9.700	4.109	-1.603	1.00	30.43
	976	CD	GLN	A	792	9.421	2.749	-2.277	1.00	31.95
25	977	OE1	GLN	A	792	8.479	2.607	-3.062	1.00	33.53
	978	NE2	GLN	A	792	10.273	1.764	-2.007	1.00	32.31
	979	N	GLU	A	793	8.886	5.301	2.907	1.00	23.72
30	980	CA	GLU	A	793	8.014	5.550	4.051	1.00	22.89
	981	C	GLU	A	793	7.949	7.041	4.400	1.00	21.58
	982	O	GLU	A	793	6.903	7.530	4.764	1.00	21.52
35	983	CB	GLU	A	793	8.460	4.728	5.273	1.00	23.65
	984	CG	GLU	A	793	8.555	3.199	5.055	1.00	25.18
	985	CD	GLU	A	793	7.383	2.406	5.651	1.00	27.08
40	986	OE1	GLU	A	793	6.207	2.735	5.351	1.00	25.97
	987	OE2	GLU	A	793	7.648	1.450	6.433	1.00	28.69
	988	N	PHE	A	794	9.042	7.784	4.274	1.00	21.26
45	989	CA	PHE	A	794	8.999	9.208	4.598	1.00	20.65
	990	C	PHE	A	794	7.929	9.863	3.759	1.00	22.26
	991	O	PHE	A	794	7.387	10.906	4.138	1.00	22.19
50	992	CB	PHE	A	794	10.334	9.890	4.323	1.00	19.81
	993	CG	PHE	A	794	11.413	9.541	5.304	1.00	19.96
	994	CD1	PHE	A	794	11.226	9.728	6.662	1.00	20.01
55	995	CD2	PHE	A	794	12.599	8.974	4.878	1.00	19.43
	996	CE1	PHE	A	794	12.206	9.347	7.566	1.00	19.86
	997	CE2	PHE	A	794	13.570	8.593	5.787	1.00	18.95
60	998	CZ	PHE	A	794	13.374	8.777	7.118	1.00	19.37
	999	N	GLY	A	795	7.688	9.270	2.585	1.00	23.81
	1000	CA	GLY	A	795	6.676	9.750	1.662	1.00	25.46
65	1001	C	GLY	A	795	5.309	9.232	2.037	1.00	26.19

TABLE 8 (continued)

	THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1002	O	GLY	A	795	4.414	10.002	2.345	1.00	27.46
	1003	N	TRP	A	796	5.181	7.912	2.081	1.00	27.45
	1004	CA	TRP	A	796	3.931	7.239	2.428	1.00	28.24
10	1005	C	TRP	A	796	3.345	7.826	3.706	1.00	29.13
	1006	O	TRP	A	796	2.132	8.026	3.801	1.00	29.87
	1007	CB	TRP	A	796	4.135	5.697	2.542	1.00	27.71
15	1008	CG	TRP	A	796	4.478	4.998	1.187	1.00	27.50
	1009	CD1	TRP	A	796	4.177	5.460	-0.079	1.00	27.17
	1010	CD2	TRP	A	796	5.208	3.763	0.985	1.00	26.97
20	1011	NE1	TRP	A	796	4.676	4.601	-1.035	1.00	27.59
	1012	CE2	TRP	A	796	5.312	3.556	-0.417	1.00	26.72
	1013	CE3	TRP	A	796	5.777	2.816	1.845	1.00	25.52
25	1014	CZ2	TRP	A	796	5.967	2.448	-0.970	1.00	25.70
	1015	CZ3	TRP	A	796	6.427	1.714	1.290	1.00	25.51
	1016	CH2	TRP	A	796	6.514	1.543	-0.106	1.00	25.42
30	1017	N	LEU	A	797	4.223	8.212	4.632	1.00	29.96
	1018	CA	LEU	A	797	3.816	8.768	5.923	1.00	29.80
	1019	C	LEU	A	797	3.864	10.260	5.991	1.00	30.39
35	1020	O	LEU	A	797	3.447	10.827	6.983	1.00	32.25
	1021	CB	LEU	A	797	4.692	8.223	7.061	1.00	28.43
	1022	CG	LEU	A	797	4.552	6.736	7.383	1.00	27.68
40	1023	CD1	LEU	A	797	5.709	6.269	8.228	1.00	27.20
	1024	CD2	LEU	A	797	3.216	6.470	8.058	1.00	26.62
	1025	N	GLN	A	798	4.415	10.908	4.978	1.00	31.03
45	1026	CA	GLN	A	798	4.518	12.360	5.005	1.00	30.93
	1027	C	GLN	A	798	5.267	12.764	6.294	1.00	30.02
	1028	O	GLN	A	798	4.716	13.460	7.147	1.00	30.51
50	1029	CB	GLN	A	798	3.117	13.030	4.964	1.00	31.58
	1030	CG	GLN	A	798	2.253	12.757	3.701	1.00	32.86
	1031	CD	GLN	A	798	0.944	13.580	3.633	1.00	32.89
55	1032	OE1	GLN	A	798	0.342	13.933	4.648	1.00	33.16
	1033	NE2	GLN	A	798	0.521	13.892	2.421	1.00	33.46
	1034	N	ILE	A	799	6.497	12.283	6.462	1.00	28.60
	1035	CA	ILE	A	799	7.277	12.634	7.648	1.00	27.76
	1036	C	ILE	A	799	7.729	14.094	7.552	1.00	28.59
	1037	O	ILE	A	799	8.181	14.552	6.496	1.00	29.81
	1038	CB	ILE	A	799	8.546	11.747	7.829	1.00	26.34

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1039	CG1	ILE	A	799	8.168	10.286	8.046	1.00	25.57
	1040	CG2	ILE	A	799	9.382	12.246	9.007	1.00	25.78
	1041	CD1	ILE	A	799	7.271	10.063	9.211	1.00	25.52
10	1042	N	THR	A	800	7.610	14.790	8.678	1.00	28.71
	1043	CA	THR	A	800	7.967	16.197	8.874	1.00	28.68
	1044	C	THR	A	800	9.475	16.347	9.116	1.00	28.69
15	1045	O	THR	A	800	10.069	15.510	9.796	1.00	29.15
	1046	CB	THR	A	800	7.202	16.718	10.142	1.00	29.24
	1047	OG1	THR	A	800	5.839	17.003	9.815	1.00	31.49
20	1048	CG2	THR	A	800	7.824	17.925	10.746	1.00	29.69
	1049	N	PRO	A	801	10.116	17.407	8.565	1.00	28.18
	1050	CA	PRO	A	801	11.555	17.600	8.780	1.00	27.74
25	1051	C	PRO	A	801	11.907	17.570	10.271	1.00	27.38
	1052	O	PRO	A	801	12.981	17.101	10.666	1.00	27.75
	1053	CB	PRO	A	801	11.797	18.983	8.178	1.00	27.08
30	1054	CG	PRO	A	801	10.908	18.956	7.002	1.00	26.58
	1055	CD	PRO	A	801	9.618	18.376	7.569	1.00	27.62
	1056	N	GLN	A	802	10.982	18.045	11.095	1.00	27.01
35	1057	CA	GLN	A	802	11.189	18.079	12.542	1.00	26.73
	1058	C	GLN	A	802	10.968	16.715	13.219	1.00	24.81
	1059	O	GLN	A	802	11.599	16.415	14.222	1.00	24.41
40	1060	CB	GLN	A	802	10.316	19.162	13.192	1.00	28.09
	1061	CG	GLN	A	802	10.582	20.596	12.692	1.00	29.79
	1062	CD	GLN	A	802	9.997	20.900	11.303	1.00	30.48
45	1063	OE1	GLN	A	802	8.948	20.381	10.918	1.00	30.36
	1064	NE2	GLN	A	802	10.660	21.782	10.571	1.00	30.57
	1065	N	GLU	A	803	10.064	15.904	12.669	1.00	23.52
50	1066	CA	GLU	A	803	9.797	14.558	13.196	1.00	21.64
	1067	C	GLU	A	803	11.067	13.784	12.923	1.00	21.04
	1068	O	GLU	A	803	11.537	13.042	13.777	1.00	20.89
55	1069	CB	GLU	A	803	8.632	13.897	12.459	1.00	20.29
	1070	CG	GLU	A	803	7.277	14.434	12.848	1.00	18.44
	1071	CD	GLU	A	803	6.147	13.786	12.119	1.00	17.84
55	1072	OE1	GLU	A	803	6.308	13.392	10.958	1.00	18.19
	1073	OE2	GLU	A	803	5.065	13.680	12.704	1.00	19.88
	1074	N	PHE	A	804	11.612	14.001	11.722	1.00	19.87
	1075	CA	PHE	A	804	12.863	13.418	11.254	1.00	19.24

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1076	C	PHE	A	804	14.034	13.802	12.157	1.00	20.31
	1077	O	PHE	A	804	14.807	12.939	12.564	1.00	21.30
	1078	CB	PHE	A	804	13.144	13.867	9.822	1.00	17.23
10	1079	CG	PHE	A	804	14.557	13.645	9.384	1.00	14.85
	1080	CD1	PHE	A	804	15.012	12.380	9.095	1.00	13.76
	1081	CD2	PHE	A	804	15.440	14.706	9.301	1.00	13.69
15	1082	CE1	PHE	A	804	16.335	12.160	8.729	1.00	13.79
	1083	CE2	PHE	A	804	16.765	14.496	8.936	1.00	13.36
	1084	CZ	PHE	A	804	17.214	13.217	8.647	1.00	12.84
20	1085	N	LEU	A	805	14.187	15.086	12.463	1.00	20.30
	1086	CA	LEU	A	805	15.271	15.503	13.339	1.00	20.09
	1087	C	LEU	A	805	15.172	14.767	14.651	1.00	19.83
25	1088	O	LEU	A	805	16.142	14.205	15.106	1.00	20.77
	1089	CB	LEU	A	805	15.250	17.008	13.582	1.00	19.58
	1090	CG	LEU	A	805	15.552	17.834	12.330	1.00	20.47
30	1091	CD1	LEU	A	805	15.704	19.281	12.707	1.00	19.84
	1092	CD2	LEU	A	805	16.816	17.343	11.670	1.00	19.41
	1093	N	CYS	A	806	13.980	14.719	15.223	1.00	20.17
35	1094	CA	CYS	A	806	13.765	14.026	16.494	1.00	21.27
	1095	C	CYS	A	806	13.938	12.515	16.378	1.00	20.36
	1096	O	CYS	A	806	14.575	11.904	17.241	1.00	20.30
40	1097	CB	CYS	A	806	12.372	14.332	17.078	1.00	22.13
	1098	SG	CYS	A	806	12.142	16.017	17.706	1.00	27.50
	1099	N	MET	A	807	13.348	11.903	15.350	1.00	19.67
45	1100	CA	MET	A	807	13.491	10.458	15.160	1.00	18.10
	1101	C	MET	A	807	14.947	10.062	14.979	1.00	17.75
	1102	O	MET	A	807	15.371	9.038	15.490	1.00	18.41
50	1103	CB	MET	A	807	12.668	9.944	13.989	1.00	17.25
	1104	CG	MET	A	807	11.195	9.877	14.279	1.00	16.70
	1105	SD	MET	A	807	10.377	9.142	12.911	1.00	19.42
55	1106	CE	MET	A	807	10.144	10.560	11.908	1.00	16.21
	1107	N	LYS	A	808	15.712	10.871	14.257	1.00	17.31
	1108	CA	LYS	A	808	17.116	10.592	14.054	1.00	16.27
55	1109	C	LYS	A	808	17.857	10.726	15.376	1.00	16.89
	1110	O	LYS	A	808	18.731	9.908	15.677	1.00	16.07
	1111	CB	LYS	A	808	17.729	11.514	12.994	1.00	15.01
	1112	CG	LYS	A	808	19.171	11.154	12.733	1.00	14.63

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1113	CD	LYS	A	808	19.679	11.569	11.371	1.00	15.42
	1114	CE	LYS	A	808	19.422	13.053	11.092	1.00	15.64
	1115	NZ	LYS	A	808	20.232	13.940	11.928	1.00	14.15
10	1116	N	ALA	A	809	17.522	11.747	16.166	1.00	16.53
	1117	CA	ALA	A	809	18.175	11.931	17.461	1.00	17.68
	1118	C	ALA	A	809	17.989	10.691	18.348	1.00	19.03
15	1119	O	ALA	A	809	18.932	10.207	18.996	1.00	20.50
	1120	CB	ALA	A	809	17.628	13.139	18.155	1.00	16.91
	1121	N	LEU	A	810	16.766	10.184	18.392	1.00	19.36
20	1122	CA	LEU	A	810	16.459	9.011	19.186	1.00	18.99
	1123	C	LEU	A	810	17.116	7.716	18.722	1.00	18.88
	1124	O	LEU	A	810	17.213	6.780	19.509	1.00	20.78
25	1125	CB	LEU	A	810	14.966	8.811	19.263	1.00	19.09
	1126	CG	LEU	A	810	14.406	9.020	20.651	1.00	20.20
	1127	CD1	LEU	A	810	12.954	8.606	20.594	1.00	21.29
30	1128	CD2	LEU	A	810	15.176	8.199	21.674	1.00	18.75
	1129	N	LEU	A	811	17.537	7.636	17.456	1.00	17.63
	1130	CA	LEU	A	811	18.215	6.447	16.959	1.00	15.58
35	1131	C	LEU	A	811	19.598	6.328	17.582	1.00	15.42
	1132	O	LEU	A	811	20.189	5.252	17.554	1.00	17.27
	1133	CB	LEU	A	811	18.346	6.456	15.438	1.00	14.70
40	1134	CG	LEU	A	811	17.148	6.107	14.574	1.00	14.14
	1135	CD1	LEU	A	811	17.511	6.408	13.164	1.00	13.66
	1136	CD2	LEU	A	811	16.744	4.632	14.746	1.00	13.62
45	1137	N	LEU	A	812	20.153	7.429	18.084	1.00	13.97
	1138	CA	LEU	A	812	21.455	7.373	18.734	1.00	12.94
	1139	C	LEU	A	812	21.330	6.658	20.098	1.00	12.97
50	1140	O	LEU	A	812	22.282	6.118	20.629	1.00	12.99
	1141	CB	LEU	A	812	22.004	8.790	18.937	1.00	12.69
	1142	CG	LEU	A	812	23.342	8.893	19.670	1.00	12.03
55	1143	CD1	LEU	A	812	24.488	8.422	18.802	1.00	12.16
	1144	CD2	LEU	A	812	23.559	10.325	20.037	1.00	13.12
	1145	N	PHE	A	813	20.136	6.681	20.662	1.00	13.55
55	1146	CA	PHE	A	813	19.859	6.064	21.950	1.00	14.19
	1147	C	PHE	A	813	18.971	4.856	21.753	1.00	14.71
	1148	O	PHE	A	813	18.058	4.618	22.530	1.00	14.79
	1149	CB	PHE	A	813	19.137	7.088	22.821	1.00	15.20

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1150	CG	PHE	A	813	19.818	8.435	22.841	1.00	16.11
1151	CD1	PHE	A	813	20.946	8.640	23.624	1.00	15.97
1152	CD2	PHE	A	813	19.349	9.472	22.036	1.00	16.07
1153	CE1	PHE	A	813	21.604	9.845	23.615	1.00	18.37
1154	CE2	PHE	A	813	19.991	10.687	22.014	1.00	17.54
1155	CZ	PHE	A	813	21.126	10.883	22.801	1.00	17.99
1156	N	SER	A	814	19.255	4.082	20.709	1.00	16.09
1157	CA	SER	A	814	18.453	2.917	20.369	1.00	15.96
1158	C	SER	A	814	19.169	1.581	20.294	1.00	16.05
1159	O	SER	A	814	18.610	0.620	19.779	1.00	17.02
1160	CB	SER	A	814	17.697	3.172	19.062	1.00	15.79
1161	OG	SER	A	814	16.640	4.087	19.274	1.00	15.51
1162	N	ILE	A	815	20.395	1.498	20.779	1.00	16.07
1163	CA	ILE	A	815	21.099	0.226	20.747	1.00	17.04
1164	C	ILE	A	815	22.172	0.187	21.826	1.00	17.86
1165	O	ILE	A	815	23.111	0.981	21.802	1.00	18.49
1166	CB	ILE	A	815	21.620	-0.086	19.325	1.00	16.75
1167	CG1	ILE	A	815	22.600	-1.245	19.341	1.00	17.01
1168	CG2	ILE	A	815	22.222	1.113	18.706	1.00	17.43
1169	CD1	ILE	A	815	22.915	-1.753	17.953	1.00	17.98
1170	N	ILE	A	816	21.994	-0.700	22.809	1.00	18.25
1171	CA	ILE	A	816	22.913	-0.804	23.947	1.00	18.91
1172	C	ILE	A	816	23.302	-2.226	24.385	1.00	20.13
1173	O	ILE	A	816	22.615	-3.184	24.040	1.00	20.43
1174	CB	ILE	A	816	22.298	-0.099	25.178	1.00	19.07
1175	CG1	ILE	A	816	20.939	-0.692	25.537	1.00	18.04
1176	CG2	ILE	A	816	22.175	1.378	24.921	1.00	17.73
1177	CD1	ILE	A	816	20.516	-0.346	26.933	1.00	17.73
1178	N	PRO	A	817	24.392	-2.385	25.180	1.00	20.85
1179	CA	PRO	A	817	24.805	-3.720	25.631	1.00	22.05
1180	C	PRO	A	817	23.706	-4.320	26.458	1.00	22.95
1181	O	PRO	A	817	22.988	-3.594	27.151	1.00	23.12
1182	CB	PRO	A	817	26.016	-3.444	26.523	1.00	21.47
1183	CG	PRO	A	817	26.554	-2.197	26.001	1.00	21.80
1184	CD	PRO	A	817	25.303	-1.373	25.730	1.00	21.00
1185	N	VAL	A	818	23.585	-5.640	26.418	1.00	24.79
1186	CA	VAL	A	818	22.544	-6.316	27.195	1.00	26.35

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1187	C	VAL	A	818	22.742	-6.047	28.692	1.00	26.79
	1188	O	VAL	A	818	21.777	-5.849	29.421	1.00	26.79
	1189	CB	VAL	A	818	22.513	-7.860	26.916	1.00	27.19
10	1190	CG1	VAL	A	818	23.864	-8.515	27.282	1.00	27.82
	1191	CG2	VAL	A	818	21.362	-8.524	27.676	1.00	27.72
	1192	N	ASP	A	819	23.992	-5.963	29.136	1.00	27.83
15	1193	CA	ASP	A	819	24.240	-5.732	30.550	1.00	29.78
	1194	C	ASP	A	819	24.377	-4.266	30.937	1.00	29.73
	1195	O	ASP	A	819	24.899	-3.930	32.007	1.00	30.00
20	1196	CB	ASP	A	819	25.406	-6.593	31.063	1.00	32.59
	1197	CG	ASP	A	819	26.747	-5.908	30.959	1.00	35.35
	1198	OD1	ASP	A	819	27.117	-5.518	29.825	1.00	38.62
25	1199	OD2	ASP	A	819	27.431	-5.776	32.011	1.00	36.18
	1200	N	GLY	A	820	23.839	-3.403	30.085	1.00	29.43
	1201	CA	GLY	A	820	23.878	-1.974	30.342	1.00	28.69
30	1202	C	GLY	A	820	25.216	-1.317	30.125	1.00	27.42
	1203	O	GLY	A	820	26.221	-1.982	29.938	1.00	26.73
	1204	N	LEU	A	821	25.208	0.010	30.135	1.00	28.29
35	1205	CA	LEU	A	821	26.410	0.831	29.947	1.00	28.64
	1206	C	LEU	A	821	26.948	1.164	31.349	1.00	28.62
	1207	O	LEU	A	821	26.341	0.747	32.342	1.00	28.84
40	1208	CB	LEU	A	821	26.023	2.110	29.195	1.00	28.29
	1209	CG	LEU	A	821	25.083	1.940	27.991	1.00	28.32
	1210	CD1	LEU	A	821	24.046	3.022	28.031	1.00	27.27
45	1211	CD2	LEU	A	821	25.831	1.953	26.653	1.00	27.18
	1212	N	LYS	A	822	28.060	1.897	31.441	1.00	28.49
	1213	CA	LYS	A	822	28.642	2.268	32.741	1.00	29.80
50	1214	C	LYS	A	822	27.621	3.016	33.587	1.00	30.25
	1215	O	LYS	A	822	27.353	2.655	34.731	1.00	31.02
	1216	CB	LYS	A	822	29.865	3.169	32.576	1.00	30.45
55	1217	CG	LYS	A	822	30.924	2.626	31.666	1.00	32.84
	1218	CD	LYS	A	822	31.517	1.345	32.194	1.00	35.27
	1219	CE	LYS	A	822	32.433	0.688	31.161	1.00	36.20
55	1220	NZ	LYS	A	822	33.498	1.623	30.710	1.00	37.22
	1221	N	ASN	A	823	27.065	4.080	33.029	1.00	29.98
	1222	CA	ASN	A	823	26.070	4.852	33.735	1.00	29.55
	1223	C	ASN	A	823	24.807	4.665	32.943	1.00	28.73

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1224	O	ASN	A	823	24.476	5.473	32.091	1.00	29.00
1225	CB	ASN	A	823	26.458	6.323	33.774	1.00	31.17
1226	CG	ASN	A	823	27.832	6.544	34.350	1.00	32.55
1227	OD1	ASN	A	823	28.787	5.856	33.985	1.00	33.56
1228	ND2	ASN	A	823	27.952	7.520	35.246	1.00	34.42
1229	N	GLN	A	824	24.127	3.562	33.199	1.00	27.99
1230	CA	GLN	A	824	22.893	3.227	32.514	1.00	27.77
1231	C	GLN	A	824	21.723	4.115	32.960	1.00	27.61
1232	O	GLN	A	824	20.747	4.275	32.226	1.00	27.58
1233	CB	GLN	A	824	22.590	1.731	32.738	1.00	28.13
1234	CG	GLN	A	824	21.343	1.158	32.077	1.00	28.93
1235	CD	GLN	A	824	21.331	1.302	30.551	1.00	30.20
1236	OE1	GLN	A	824	22.300	0.976	29.855	1.00	30.02
1237	NE2	GLN	A	824	20.211	1.775	30.028	1.00	29.72
1238	N	LYS	A	825	21.833	4.752	34.122	1.00	27.13
1239	CA	LYS	A	825	20.742	5.590	34.595	1.00	26.37
1240	C	LYS	A	825	20.679	6.917	33.876	1.00	24.74
1241	O	LYS	A	825	19.625	7.518	33.799	1.00	25.30
1242	CB	LYS	A	825	20.815	5.802	36.113	1.00	28.08
1243	CG	LYS	A	825	19.430	5.823	36.792	1.00	31.02
1244	CD	LYS	A	825	19.493	5.693	38.335	1.00	33.41
1245	CE	LYS	A	825	18.086	5.725	39.002	1.00	34.57
1246	NZ	LYS	A	825	17.196	4.516	38.739	1.00	35.55
1247	N	PHE	A	826	21.794	7.375	33.330	1.00	24.06
1248	CA	PHE	A	826	21.830	8.646	32.597	1.00	23.44
1249	C	PHE	A	826	21.344	8.463	31.178	1.00	21.78
1250	O	PHE	A	826	20.808	9.380	30.568	1.00	21.42
1251	CB	PHE	A	826	23.247	9.191	32.573	1.00	25.61
1252	CG	PHE	A	826	23.768	9.527	33.930	1.00	28.86
1253	CD1	PHE	A	826	22.916	10.067	34.890	1.00	29.49
1254	CD2	PHE	A	826	25.091	9.284	34.268	1.00	29.08
1255	CE1	PHE	A	826	23.373	10.356	36.156	1.00	29.57
1256	CE2	PHE	A	826	25.551	9.571	35.533	1.00	29.80
1257	CZ	PHE	A	826	24.688	10.108	36.479	1.00	30.14
1258	N	PHE	A	827	21.581	7.277	30.636	1.00	20.42
1259	CA	PHE	A	827	21.145	6.937	29.299	1.00	18.74
1260	C	PHE	A	827	19.627	6.778	29.277	1.00	19.19

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1261	O	PHE	A	827	18.962	7.183	28.331	1.00	18.79
	1262	CB	PHE	A	827	21.814	5.644	28.857	1.00	17.62
	1263	CG	PHE	A	827	21.238	5.083	27.610	1.00	16.77
10	1264	CD1	PHE	A	827	21.780	5.412	26.380	1.00	16.74
	1265	CD2	PHE	A	827	20.123	4.261	27.656	1.00	16.46
	1266	CE1	PHE	A	827	21.225	4.939	25.212	1.00	16.50
15	1267	CE2	PHE	A	827	19.555	3.782	26.491	1.00	17.41
	1268	CZ	PHE	A	827	20.105	4.120	25.266	1.00	16.35
	1269	N	ASP	A	828	19.079	6.150	30.312	1.00	20.42
20	1270	CA	ASP	A	828	17.638	5.943	30.421	1.00	21.69
	1271	C	ASP	A	828	16.931	7.287	30.572	1.00	21.41
	1272	O	ASP	A	828	15.835	7.487	30.070	1.00	21.87
25	1273	CB	ASP	A	828	17.325	5.045	31.633	1.00	23.37
	1274	CG	ASP	A	828	17.885	3.627	31.487	1.00	24.46
	1275	OD1	ASP	A	828	17.900	3.095	30.365	1.00	26.34
30	1276	OD2	ASP	A	828	18.296	3.023	32.501	1.00	26.77
	1277	N	GLU	A	829	17.552	8.187	31.313	1.00	22.11
	1278	CA	GLU	A	829	17.005	9.510	31.533	1.00	23.92
35	1279	C	GLU	A	829	17.011	10.166	30.174	1.00	22.78
	1280	O	GLU	A	829	15.963	10.539	29.656	1.00	22.06
	1281	CB	GLU	A	829	17.910	10.309	32.499	1.00	27.77
40	1282	CG	GLU	A	829	18.168	11.823	32.130	1.00	32.20
	1283	CD	GLU	A	829	19.650	12.266	32.334	1.00	35.29
	1284	OE1	GLU	A	829	20.005	12.655	33.482	1.00	37.06
45	1285	OE2	GLU	A	829	20.463	12.217	31.360	1.00	34.89
	1286	N	LEU	A	830	18.201	10.200	29.575	1.00	22.21
	1287	CA	LEU	A	830	18.437	10.812	28.272	1.00	22.14
50	1288	C	LEU	A	830	17.499	10.318	27.191	1.00	22.74
	1289	O	LEU	A	830	16.874	11.114	26.481	1.00	23.35
	1290	CB	LEU	A	830	19.885	10.575	27.852	1.00	21.24
55	1291	CG	LEU	A	830	20.415	11.572	26.833	1.00	21.76
	1292	CD1	LEU	A	830	20.037	13.004	27.215	1.00	21.40
	1293	CD2	LEU	A	830	21.895	11.429	26.752	1.00	22.34
55	1294	N	ARG	A	831	17.400	9.002	27.079	1.00	22.23
	1295	CA	ARG	A	831	16.559	8.352	26.097	1.00	22.37
	1296	C	ARG	A	831	15.086	8.667	26.302	1.00	22.46
	1297	O	ARG	A	831	14.354	8.964	25.351	1.00	22.89

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1298	CB	ARG	A	831	16.780	6.849	26.186	1.00	22.50
1299	CG	ARG	A	831	15.957	6.087	25.219	1.00	22.59
1300	CD	ARG	A	831	16.130	4.600	25.375	1.00	23.29
1301	NE	ARG	A	831	15.921	3.972	24.074	1.00	25.50
1302	CZ	ARG	A	831	14.738	3.800	23.491	1.00	24.36
1303	NH1	ARG	A	831	13.632	4.173	24.096	1.00	25.37
1304	NH2	ARG	A	831	14.676	3.366	22.250	1.00	24.31
1305	N	MET	A	832	14.655	8.593	27.550	1.00	22.76
1306	CA	MET	A	832	13.276	8.859	27.923	1.00	22.91
1307	C	MET	A	832	12.879	10.262	27.513	1.00	23.47
1308	O	MET	A	832	11.740	10.512	27.097	1.00	23.79
1309	CB	MET	A	832	13.126	8.762	29.429	1.00	23.88
1310	CG	MET	A	832	11.739	9.050	29.870	1.00	24.65
1311	SD	MET	A	832	11.693	9.332	31.596	1.00	29.43
1312	CE	MET	A	832	10.059	10.026	31.651	1.00	29.67
1313	N	ASN	A	833	13.782	11.198	27.768	1.00	23.63
1314	CA	ASN	A	833	13.562	12.599	27.423	1.00	23.80
1315	C	ASN	A	833	13.403	12.761	25.905	1.00	23.94
1316	O	ASN	A	833	12.463	13.397	25.445	1.00	24.48
1317	CB	ASN	A	833	14.676	13.482	28.013	1.00	23.64
1318	CG	ASN	A	833	14.532	13.679	29.544	1.00	23.87
1319	OD1	ASN	A	833	15.519	13.864	30.270	1.00	23.24
1320	ND2	ASN	A	833	13.293	13.628	30.030	1.00	24.57
1321	N	TYR	A	834	14.240	12.093	25.123	1.00	23.69
1322	CA	TYR	A	834	14.121	12.165	23.673	1.00	24.70
1323	C	TYR	A	834	12.809	11.574	23.128	1.00	24.43
1324	O	TYR	A	834	12.297	12.006	22.082	1.00	24.26
1325	CB	TYR	A	834	15.340	11.532	23.007	1.00	25.39
1326	CG	TYR	A	834	16.491	12.489	22.872	1.00	25.49
1327	CD1	TYR	A	834	16.802	13.051	21.635	1.00	26.75
1328	CD2	TYR	A	834	17.239	12.869	23.986	1.00	26.00
1329	CE1	TYR	A	834	17.828	13.975	21.502	1.00	27.67
1330	CE2	TYR	A	834	18.268	13.791	23.873	1.00	26.69
1331	CZ	TYR	A	834	18.558	14.341	22.624	1.00	28.15
1332	OH	TYR	A	834	19.571	15.263	22.497	1.00	28.86
1333	N	ILE	A	835	12.260	10.599	23.843	1.00	24.33
1334	CA	ILE	A	835	11.004	9.991	23.450	1.00	23.48

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1335	C	ILE	A	835	9.893	10.977	23.687	1.00	25.05
	1336	O	ILE	A	835	8.972	11.061	22.889	1.00	26.24
	1337	CB	ILE	A	835	10.724	8.727	24.235	1.00	21.33
10	1338	CG1	ILE	A	835	11.657	7.624	23.756	1.00	20.40
	1339	CG2	ILE	A	835	9.297	8.308	24.054	1.00	19.87
	1340	CD1	ILE	A	835	11.684	6.400	24.655	1.00	21.05
15	1341	N	LYS	A	836	9.998	11.738	24.771	1.00	26.82
	1342	CA	LYS	A	836	9.006	12.747	25.137	1.00	28.28
	1343	C	LYS	A	836	9.030	13.919	24.164	1.00	28.39
20	1344	O	LYS	A	836	7.997	14.545	23.946	1.00	29.09
	1345	CB	LYS	A	836	9.245	13.281	26.556	1.00	29.95
	1346	CG	LYS	A	836	9.115	12.252	27.712	1.00	32.62
25	1347	CD	LYS	A	836	7.690	11.672	27.901	1.00	33.04
	1348	CE	LYS	A	836	7.575	10.238	27.344	1.00	34.32
	1349	NZ	LYS	A	836	8.559	9.259	27.942	1.00	32.90
30	1350	N	GLU	A	837	10.194	14.249	23.606	1.00	28.61
	1351	CA	GLU	A	837	10.276	15.351	22.643	1.00	28.70
	1352	C	GLU	A	837	9.666	14.907	21.321	1.00	28.92
35	1353	O	GLU	A	837	9.041	15.699	20.626	1.00	28.40
	1354	CB	GLU	A	837	11.715	15.824	22.439	1.00	29.34
	1355	CG	GLU	A	837	12.305	16.584	23.627	1.00	32.13
40	1356	CD	GLU	A	837	11.553	17.887	23.971	1.00	34.30
	1357	OE1	GLU	A	837	11.612	18.303	25.157	1.00	34.18
	1358	OE2	GLU	A	837	10.925	18.503	23.063	1.00	35.58
45	1359	N	LEU	A	838	9.826	13.631	20.991	1.00	29.32
	1360	CA	LEU	A	838	9.250	13.092	19.774	1.00	30.90
	1361	C	LEU	A	838	7.740	13.211	19.884	1.00	32.66
50	1362	O	LEU	A	838	7.076	13.706	18.983	1.00	32.60
	1363	CB	LEU	A	838	9.614	11.622	19.592	1.00	30.44
	1364	CG	LEU	A	838	8.810	10.983	18.460	1.00	30.56
55	1365	CD1	LEU	A	838	9.077	11.728	17.151	1.00	30.31
	1366	CD2	LEU	A	838	9.166	9.533	18.330	1.00	30.00
	1367	N	ASP	A	839	7.186	12.724	20.979	1.00	34.82
55	1368	CA	ASP	A	839	5.755	12.823	21.162	1.00	37.61
	1369	C	ASP	A	839	5.338	14.293	21.187	1.00	38.83
	1370	O	ASP	A	839	4.285	14.645	20.672	1.00	39.02
	1371	CB	ASP	A	839	5.331	12.117	22.449	1.00	39.22

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1372	CG	ASP	A	839	3.816	11.952	22.557	1.00	41.54
1373	OD1	ASP	A	839	3.249	12.375	23.592	1.00	43.10
1374	OD2	ASP	A	839	3.192	11.400	21.613	1.00	42.60
1375	N	ARG	A	840	6.195	15.151	21.731	1.00	40.51
1376	CA	ARG	A	840	5.916	16.580	21.828	1.00	42.20
1377	C	ARG	A	840	5.776	17.220	20.457	1.00	43.27
1378	O	ARG	A	840	4.860	18.004	20.232	1.00	43.50
1379	CB	ARG	A	840	7.032	17.289	22.610	1.00	43.32
1380	CG	ARG	A	840	6.657	18.639	23.261	1.00	45.47
1381	CD	ARG	A	840	6.945	19.881	22.401	1.00	46.95
1382	NE	ARG	A	840	8.319	20.371	22.542	1.00	48.57
1383	CZ	ARG	A	840	9.066	20.823	21.533	1.00	49.57
1384	NH1	ARG	A	840	8.580	20.860	20.294	1.00	49.89
1385	NH2	ARG	A	840	10.314	21.220	21.755	1.00	49.90
1386	N	ILE	A	841	6.663	16.876	19.528	1.00	44.53
1387	CA	ILE	A	841	6.600	17.483	18.211	1.00	46.22
1388	C	ILE	A	841	5.534	16.913	17.286	1.00	48.04
1389	O	ILE	A	841	5.472	17.272	16.109	1.00	48.90
1390	CB	ILE	A	841	7.983	17.572	17.510	1.00	45.82
1391	CG1	ILE	A	841	8.383	16.237	16.918	1.00	46.46
1392	CG2	ILE	A	841	9.044	18.078	18.463	1.00	46.40
1393	CD1	ILE	A	841	8.064	16.150	15.463	1.00	45.92
1394	N	ILE	A	842	4.737	15.976	17.786	1.00	49.91
1395	CA	ILE	A	842	3.632	15.446	16.990	1.00	51.38
1396	C	ILE	A	842	2.384	16.003	17.659	1.00	52.63
1397	O	ILE	A	842	1.509	16.551	16.999	1.00	52.38
1398	CB	ILE	A	842	3.577	13.878	16.889	1.00	51.11
1399	CG1	ILE	A	842	4.523	13.192	17.870	1.00	50.67
1400	CG2	ILE	A	842	3.917	13.445	15.482	1.00	51.75
1401	CD1	ILE	A	842	4.691	11.701	17.619	1.00	49.36
1402	N	ALA	A	843	2.356	15.939	18.986	1.00	54.81
1403	CA	ALA	A	843	1.242	16.456	19.761	1.00	57.24
1404	C	ALA	A	843	1.215	17.962	19.557	1.00	59.28
1405	O	ALA	A	843	1.847	18.704	20.304	1.00	59.69
1406	CB	ALA	A	843	1.424	16.129	21.247	1.00	56.69
1407	N	CYS	A	844	0.560	18.391	18.481	1.00	61.60
1408	CA	CYS	A	844	0.402	19.810	18.130	1.00	63.67

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1409	C	CYS	A	844	-0.441	19.854	16.848	1.00	64.63
	1410	O	CYS	A	844	-1.618	19.471	16.889	1.00	64.70
	1411	CB	CYS	A	844	1.766	20.536	17.979	1.00	64.05
10	1412	SG	CYS	A	844	2.751	20.268	16.470	1.00	65.30
	1413	N	LYS	A	845	0.136	20.332	15.738	1.00	65.65
	1414	CA	LYS	A	845	-0.545	20.374	14.439	1.00	65.96
15	1415	C	LYS	A	845	-0.079	19.165	13.644	1.00	66.49
	1416	O	LYS	A	845	-0.675	18.829	12.620	1.00	66.85
	1417	CB	LYS	A	845	-0.195	21.639	13.684	1.00	65.80
20	1418	N	ARG	A	846	0.998	18.533	14.127	1.00	66.74
	1419	CA	ARG	A	846	1.601	17.343	13.511	1.00	66.90
	1420	C	ARG	A	846	0.984	16.074	14.086	1.00	66.88
25	1421	O	ARG	A	846	1.675	15.092	14.345	1.00	66.35
	1422	CB	ARG	A	846	3.110	17.337	13.730	1.00	66.74
	1423	N	LYS	A	847	-0.325	16.141	14.291	1.00	67.27
30	1424	CA	LYS	A	847	-1.162	15.076	14.826	1.00	67.87
	1425	C	LYS	A	847	-2.420	15.816	15.251	1.00	68.35
	1426	O	LYS	A	847	-2.432	17.046	15.278	1.00	68.33
35	1427	CB	LYS	A	847	-0.515	14.407	16.033	1.00	68.14
	1428	N	ASN	A	848	-3.468	15.079	15.597	1.00	69.11
	1429	CA	ASN	A	848	-4.728	15.685	16.016	1.00	69.71
40	1430	C	ASN	A	848	-5.737	14.586	16.340	1.00	70.20
	1431	O	ASN	A	848	-5.342	13.474	16.720	1.00	70.21
	1432	CB	ASN	A	848	-5.272	16.598	14.907	1.00	69.68
45	1433	N	PRO	A	849	-7.021	14.914	16.146	1.00	70.54
	1434	CA	PRO	A	849	-8.185	14.043	16.374	1.00	70.31
	1435	C	PRO	A	849	-7.856	12.661	16.920	1.00	69.92
50	1436	O	PRO	A	849	-7.665	12.492	18.130	1.00	70.12
	1437	CB	PRO	A	849	-9.014	13.929	15.079	1.00	70.65
	1438	N	THR	A	850	-7.808	11.680	16.020	1.00	69.47
55	1439	CA	THR	A	850	-7.473	10.304	16.377	1.00	68.74
	1440	C	THR	A	850	-6.061	10.015	15.845	1.00	67.76
	1441	O	THR	A	850	-5.590	8.867	15.864	1.00	67.27
55	1442	CB	THR	A	850	-8.494	9.331	15.774	1.00	68.95
	1443	N	SER	A	851	-5.391	11.077	15.388	1.00	66.46
	1444	CA	SER	A	851	-4.046	10.962	14.846	1.00	65.28
	1445	C	SER	A	851	-3.023	10.710	15.944	1.00	64.16

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1446	O	SER	A	851	-2.426	9.639	15.969	1.00	64.16
1447	CB	SER	A	851	-3.664	12.200	14.018	1.00	65.24
1448	OG	SER	A	851	-2.405	12.037	13.369	1.00	65.05
1449	N	CYS	A	852	-2.873	11.651	16.879	1.00	62.68
1450	CA	CYS	A	852	-1.901	11.526	17.974	1.00	60.96
1451	C	CYS	A	852	-1.480	10.102	18.388	1.00	59.71
1452	O	CYS	A	852	-0.282	9.800	18.422	1.00	59.67
1453	CB	CYS	A	852	-2.353	12.333	19.191	1.00	61.34
1454	SG	CYS	A	852	-1.712	14.024	19.216	1.00	62.06
1455	N	SER	A	853	-2.440	9.223	18.678	1.00	57.85
1456	CA	SER	A	853	-2.109	7.847	19.053	1.00	55.45
1457	C	SER	A	853	-1.610	7.052	17.847	1.00	53.09
1458	O	SER	A	853	-0.601	6.346	17.942	1.00	53.22
1459	CB	SER	A	853	-3.308	7.133	19.686	1.00	56.27
1460	OG	SER	A	853	-3.480	7.522	21.038	1.00	57.65
1461	N	ARG	A	854	-2.304	7.172	16.719	1.00	49.75
1462	CA	ARG	A	854	-1.924	6.462	15.500	1.00	46.39
1463	C	ARG	A	854	-0.564	6.962	14.967	1.00	43.72
1464	O	ARG	A	854	0.294	6.164	14.564	1.00	43.80
1465	CB	ARG	A	854	-3.021	6.634	14.443	1.00	47.23
1466	CG	ARG	A	854	-2.747	5.970	13.105	1.00	48.09
1467	CD	ARG	A	854	-2.985	6.943	11.940	1.00	49.85
1468	NE	ARG	A	854	-4.340	7.500	11.936	1.00	51.11
1469	CZ	ARG	A	854	-4.911	8.122	10.904	1.00	51.20
1470	NH1	ARG	A	854	-4.261	8.290	9.755	1.00	51.32
1471	NH2	ARG	A	854	-6.153	8.567	11.021	1.00	51.21
1472	N	ARG	A	855	-0.360	8.273	15.019	1.00	39.68
1473	CA	ARG	A	855	0.860	8.926	14.558	1.00	36.58
1474	C	ARG	A	855	2.106	8.454	15.306	1.00	35.02
1475	O	ARG	A	855	3.180	8.326	14.723	1.00	34.97
1476	CB	ARG	A	855	0.713	10.439	14.734	1.00	36.42
1477	CG	ARG	A	855	1.801	11.264	14.082	1.00	34.79
1478	CD	ARG	A	855	1.724	11.109	12.594	1.00	32.86
1479	NE	ARG	A	855	2.869	11.699	11.907	1.00	30.54
1480	CZ	ARG	A	855	3.030	11.655	10.590	1.00	29.61
1481	NH1	ARG	A	855	2.130	11.051	9.831	1.00	28.88
1482	NH2	ARG	A	855	4.085	12.219	10.028	1.00	29.20

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1483	N	PHE	A	856	1.973	8.239	16.609	1.00	33.30
	1484	CA	PHE	A	856	3.086	7.786	17.428	1.00	31.21
	1485	C	PHE	A	856	3.308	6.290	17.254	1.00	30.61
10	1486	O	PHE	A	856	4.420	5.803	17.424	1.00	30.75
	1487	CB	PHE	A	856	2.846	8.128	18.895	1.00	30.24
	1488	CG	PHE	A	856	4.058	7.977	19.755	1.00	30.06
15	1489	CD1	PHE	A	856	5.022	8.972	19.787	1.00	29.34
	1490	CD2	PHE	A	856	4.241	6.829	20.536	1.00	29.33
	1491	CE1	PHE	A	856	6.150	8.832	20.580	1.00	29.36
20	1492	CE2	PHE	A	856	5.364	6.676	21.335	1.00	28.86
	1493	CZ	PHE	A	856	6.325	7.680	21.357	1.00	29.62
	1494	N	TYR	A	857	2.258	5.543	16.943	1.00	29.79
25	1495	CA	TYR	A	857	2.446	4.118	16.725	1.00	29.79
	1496	C	TYR	A	857	3.206	3.929	15.419	1.00	29.44
	1497	O	TYR	A	857	4.135	3.125	15.371	1.00	29.44
30	1498	CB	TYR	A	857	1.116	3.365	16.660	1.00	30.78
	1499	CG	TYR	A	857	1.254	1.871	16.396	1.00	32.21
	1500	CD1	TYR	A	857	1.425	0.972	17.442	1.00	32.75
35	1501	CD2	TYR	A	857	1.208	1.362	15.098	1.00	33.36
	1502	CE1	TYR	A	857	1.548	-0.401	17.215	1.00	34.60
	1503	CE2	TYR	A	857	1.331	-0.011	14.854	1.00	34.67
40	1504	CZ	TYR	A	857	1.503	-0.887	15.918	1.00	35.61
	1505	OH	TYR	A	857	1.652	-2.244	15.697	1.00	36.96
	1506	N	GLN	A	858	2.847	4.685	14.376	1.00	28.32
45	1507	CA	GLN	A	858	3.533	4.537	13.087	1.00	28.06
	1508	C	GLN	A	858	4.967	5.077	13.037	1.00	26.56
	1509	O	GLN	A	858	5.820	4.525	12.332	1.00	26.58
50	1510	CB	GLN	A	858	2.675	5.020	11.890	1.00	28.98
	1511	CG	GLN	A	858	1.970	6.384	12.029	1.00	31.65
	1512	CD	GLN	A	858	0.781	6.569	11.059	1.00	32.26
55	1513	OE1	GLN	A	858	0.385	7.700	10.724	1.00	32.11
	1514	NE2	GLN	A	858	0.210	5.458	10.617	1.00	32.79
	1515	N	LEU	A	859	5.266	6.101	13.825	1.00	24.64
55	1516	CA	LEU	A	859	6.622	6.632	13.832	1.00	22.82
	1517	C	LEU	A	859	7.545	5.705	14.613	1.00	20.92
	1518	O	LEU	A	859	8.694	5.486	14.222	1.00	20.35
	1519	CB	LEU	A	859	6.675	8.067	14.395	1.00	23.93

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1520	CG	LEU	A	859	6.054	9.243	13.617	1.00	23.18
	1521	CD1	LEU	A	859	6.616	10.541	14.156	1.00	23.42
	1522	CD2	LEU	A	859	6.363	9.137	12.173	1.00	22.30
10	1523	N	THR	A	860	7.030	5.124	15.691	1.00	20.30
	1524	CA	THR	A	860	7.821	4.195	16.505	1.00	20.14
	1525	C	THR	A	860	7.969	2.855	15.765	1.00	20.30
15	1526	O	THR	A	860	8.922	2.108	15.985	1.00	20.28
	1527	CB	THR	A	860	7.215	3.957	17.905	1.00	18.65
	1528	OG1	THR	A	860	5.849	3.551	17.797	1.00	18.55
20	1529	CG2	THR	A	860	7.314	5.196	18.734	1.00	18.12
	1530	N	LYS	A	861	7.040	2.600	14.851	1.00	21.02
	1531	CA	LYS	A	861	7.046	1.411	14.034	1.00	21.82
25	1532	C	LYS	A	861	8.040	1.642	12.895	1.00	21.28
	1533	O	LYS	A	861	8.781	0.750	12.510	1.00	21.01
	1534	CB	LYS	A	861	5.649	1.178	13.475	1.00	23.82
30	1535	CG	LYS	A	861	5.375	-0.268	13.110	1.00	26.71
	1536	CD	LYS	A	861	5.015	-1.106	14.321	1.00	28.40
	1537	CE	LYS	A	861	4.924	-2.587	13.922	1.00	30.14
35	1538	NZ	LYS	A	861	4.542	-3.514	15.050	1.00	31.53
	1539	N	LEU	A	862	8.093	2.863	12.389	1.00	21.49
	1540	CA	LEU	A	862	9.021	3.192	11.311	1.00	21.32
40	1541	C	LEU	A	862	10.438	3.181	11.854	1.00	21.15
	1542	O	LEU	A	862	11.386	2.884	11.133	1.00	22.30
	1543	CB	LEU	A	862	8.713	4.577	10.731	1.00	22.14
45	1544	CG	LEU	A	862	9.816	5.281	9.921	1.00	21.98
	1545	CD1	LEU	A	862	10.022	4.563	8.622	1.00	22.72
	1546	CD2	LEU	A	862	9.456	6.726	9.670	1.00	22.58
50	1547	N	LEU	A	863	10.596	3.602	13.105	1.00	20.71
	1548	CA	LEU	A	863	11.906	3.625	13.749	1.00	18.90
	1549	C	LEU	A	863	12.462	2.218	14.004	1.00	18.08
55	1550	O	LEU	A	863	13.676	1.984	13.895	1.00	17.06
	1551	CB	LEU	A	863	11.827	4.423	15.040	1.00	18.78
	1552	CG	LEU	A	863	11.890	5.931	14.863	1.00	18.02
	1553	CD1	LEU	A	863	12.103	6.545	16.230	1.00	19.67
	1554	CD2	LEU	A	863	13.049	6.291	13.944	1.00	16.59
	1555	N	ASP	A	864	11.592	1.307	14.436	1.00	18.33
	1556	CA	ASP	A	864	11.985	-0.088	14.642	1.00	19.28

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1557	C	ASP	A	864	12.467	-0.692	13.321	1.00	19.06
	1558	O	ASP	A	864	13.377	-1.519	13.298	1.00	18.82
	1559	CB	ASP	A	864	10.797	-0.917	15.143	1.00	19.27
10	1560	CG	ASP	A	864	10.525	-0.727	16.620	1.00	19.92
	1561	OD1	ASP	A	864	11.256	0.045	17.271	1.00	20.94
	1562	OD2	ASP	A	864	9.577	-1.364	17.116	1.00	19.39
15	1563	N	SER	A	865	11.847	-0.263	12.222	1.00	19.90
	1564	CA	SER	A	865	12.202	-0.764	10.894	1.00	19.17
	1565	C	SER	A	865	13.634	-0.507	10.489	1.00	18.01
20	1566	O	SER	A	865	14.213	-1.294	9.765	1.00	18.93
	1567	CB	SER	A	865	11.226	-0.289	9.798	1.00	18.59
	1568	OG	SER	A	865	11.167	1.123	9.613	1.00	19.91
25	1569	N	VAL	A	866	14.257	0.535	11.004	1.00	17.08
	1570	CA	VAL	A	866	15.619	0.747	10.589	1.00	15.20
	1571	C	VAL	A	866	16.564	-0.260	11.194	1.00	14.83
30	1572	O	VAL	A	866	17.625	-0.518	10.641	1.00	14.66
	1573	CB	VAL	A	866	16.093	2.211	10.783	1.00	15.01
	1574	CG1	VAL	A	866	14.982	3.081	11.320	1.00	13.81
35	1575	CG2	VAL	A	866	17.344	2.280	11.574	1.00	13.41
	1576	N	GLN	A	867	16.168	-0.873	12.302	1.00	15.12
	1577	CA	GLN	A	867	17.031	-1.849	12.977	1.00	15.64
40	1578	C	GLN	A	867	17.358	-3.143	12.233	1.00	14.54
	1579	O	GLN	A	867	18.487	-3.594	12.271	1.00	15.92
	1580	CB	GLN	A	867	16.508	-2.155	14.374	1.00	16.10
45	1581	CG	GLN	A	867	16.526	-0.968	15.315	1.00	16.35
	1582	CD	GLN	A	867	17.910	-0.474	15.672	1.00	17.91
	1583	OE1	GLN	A	867	18.924	-1.175	15.510	1.00	17.76
50	1584	NE2	GLN	A	867	17.958	0.750	16.201	1.00	17.53
	1585	N	PRO	A	868	16.364	-3.809	11.634	1.00	14.35
	1586	CA	PRO	A	868	16.630	-5.040	10.886	1.00	13.73
55	1587	C	PRO	A	868	17.500	-4.704	9.674	1.00	13.45
	1588	O	PRO	A	868	18.341	-5.497	9.254	1.00	14.77
	1589	CB	PRO	A	868	15.232	-5.465	10.415	1.00	14.35
60	1590	CG	PRO	A	868	14.331	-4.928	11.438	1.00	14.42
	1591	CD	PRO	A	868	14.914	-3.555	11.696	1.00	15.17
	1592	N	ILE	A	869	17.289	-3.514	9.113	1.00	13.49
65	1593	CA	ILE	A	869	18.043	-3.044	7.970	1.00	12.06

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1594	C	ILE	A	869	19.458	-2.818	8.411	11.70
	1595	O	ILE	A	869	20.356	-3.302	7.755	13.01
	1596	CB	ILE	A	869	17.447	-1.740	7.358	12.53
10	1597	CG1	ILE	A	869	15.998	-1.973	6.928	12.25
	1598	CG2	ILE	A	869	18.272	-1.307	6.175	12.44
	1599	CD1	ILE	A	869	15.258	-0.746	6.432	11.91
	1600	N	ALA	A	870	19.655	-2.254	9.610	12.19
15	1601	CA	ALA	A	870	21.007	-1.993	10.110	11.52
	1602	C	ALA	A	870	21.758	-3.287	10.350	12.90
	1603	O	ALA	A	870	22.955	-3.374	10.074	13.99
20	1604	CB	ALA	A	870	20.971	-1.189	11.375	10.62
	1605	N	ARG	A	871	21.082	-4.262	10.962	14.67
	1606	CA	ARG	A	871	21.659	-5.577	11.226	15.30
	1607	C	ARG	A	871	22.119	-6.287	9.939	16.18
25	1608	O	ARG	A	871	23.216	-6.846	9.897	16.90
	1609	CB	ARG	A	871	20.668	-6.465	11.970	16.99
	1610	CG	ARG	A	871	21.317	-7.789	12.304	20.44
30	1611	CD	ARG	A	871	20.552	-8.755	13.190	22.19
	1612	NE	ARG	A	871	21.529	-9.736	13.678	25.05
	1613	CZ	ARG	A	871	22.248	-9.581	14.785	24.87
	1614	NH1	ARG	A	871	22.085	-8.513	15.553	26.86
35	1615	NH2	ARG	A	871	23.221	-10.425	15.059	27.12
	1616	N	GLU	A	872	21.300	-6.256	8.886	17.08
	1617	CA	GLU	A	872	21.669	-6.874	7.595	17.70
40	1618	C	GLU	A	872	22.961	-6.229	7.064	16.22
	1619	O	GLU	A	872	23.826	-6.892	6.504	16.64
	1620	CB	GLU	A	872	20.546	-6.670	6.578	20.21
	1621	CG	GLU	A	872	20.070	-7.920	5.827	27.32
45	1622	CD	GLU	A	872	19.041	-7.600	4.715	31.24
	1623	OE1	GLU	A	872	19.199	-8.069	3.544	32.65
	1624	OE2	GLU	A	872	18.068	-6.867	5.018	33.14
50	1625	N	LEU	A	873	23.109	-4.927	7.254	15.48
	1626	CA	LEU	A	873	24.304	-4.230	6.781	13.64
	1627	C	LEU	A	873	25.489	-4.510	7.662	13.26
	1628	O	LEU	A	873	26.621	-4.541	7.185	12.91
55	1629	CB	LEU	A	873	24.040	-2.718	6.664	13.09
	1630	CG	LEU	A	873	22.957	-2.359	5.640	12.60

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1631	CD1	LEU	A	873	22.396	-0.985	5.856	13.12
	1632	CD2	LEU	A	873	23.511	-2.529	4.229	12.29
	1633	N	HIS	A	874	25.237	-4.688	8.960	14.96
10	1634	CA	HIS	A	874	26.297	-5.011	9.935	15.73
	1635	C	HIS	A	874	26.945	-6.342	9.549	16.66
	1636	O	HIS	A	874	28.171	-6.454	9.539	16.68
	1637	CB	HIS	A	874	25.735	-5.154	11.351	14.09
15	1638	CG	HIS	A	874	25.513	-3.860	12.062	13.53
	1639	ND1	HIS	A	874	24.365	-3.588	12.771	12.74
	1640	CD2	HIS	A	874	26.303	-2.769	12.204	12.74
20	1641	CE1	HIS	A	874	24.451	-2.397	13.313	11.45
	1642	NE2	HIS	A	874	25.616	-1.878	12.990	10.87
	1643	N	GLN	A	875	26.122	-7.356	9.268	18.67
25	1644	CA	GLN	A	875	26.635	-8.674	8.853	19.45
	1645	C	GLN	A	875	27.324	-8.521	7.491	18.37
	1646	O	GLN	A	875	28.428	-9.022	7.294	18.65
	1647	CB	GLN	A	875	25.507	-9.726	8.779	21.56
30	1648	CG	GLN	A	875	25.566	-10.875	9.864	25.76
	1649	CD	GLN	A	875	26.681	-11.938	9.671	26.74
	1650	OE1	GLN	A	875	27.871	-11.624	9.654	27.36
35	1651	NE2	GLN	A	875	26.285	-13.204	9.589	27.93
	1652	N	PHE	A	876	26.737	-7.724	6.597	18.47
	1653	CA	PHE	A	876	27.338	-7.515	5.280	18.22
	1654	C	PHE	A	876	28.689	-6.871	5.403	17.76
40	1655	O	PHE	A	876	29.687	-7.412	4.920	17.95
	1656	CB	PHE	A	876	26.453	-6.641	4.377	19.25
	1657	CG	PHE	A	876	26.966	-6.506	2.954	19.63
45	1658	CD1	PHE	A	876	28.038	-5.675	2.657	18.97
	1659	CD2	PHE	A	876	26.380	-7.226	1.917	19.90
	1660	CE1	PHE	A	876	28.519	-5.558	1.343	20.30
	1661	CE2	PHE	A	876	26.857	-7.113	0.597	20.70
50	1662	CZ	PHE	A	876	27.926	-6.281	0.310	18.82
	1663	N	THR	A	877	28.741	-5.732	6.086	17.85
	1664	CA	THR	A	877	30.002	-5.024	6.215	17.77
55	1665	C	THR	A	877	31.040	-5.884	6.900	17.52
	1666	O	THR	A	877	32.208	-5.849	6.514	16.51
	1667	CB	THR	A	877	29.855	-3.641	6.915	18.24

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1668	OG1	THR	A	877	30.954	-2.808	6.525	1.00	19.13
1669	CG2	THR	A	877	29.868	-3.765	8.444	1.00	17.92
1670	N	PHE	A	878	30.634	-6.610	7.943	1.00	18.06
1671	CA	PHE	A	878	31.559	-7.501	8.651	1.00	19.20
1672	C	PHE	A	878	32.176	-8.567	7.725	1.00	18.91
1673	O	PHE	A	878	33.400	-8.724	7.670	1.00	17.63
1674	CB	PHE	A	878	30.863	-8.201	9.805	1.00	19.53
1675	CG	PHE	A	878	31.731	-9.220	10.484	1.00	20.60
1676	CD1	PHE	A	878	32.681	-8.829	11.414	1.00	19.88
1677	CD2	PHE	A	878	31.623	-10.575	10.150	1.00	20.59
1678	CE1	PHE	A	878	33.518	-9.774	12.008	1.00	22.10
1679	CE2	PHE	A	878	32.454	-11.532	10.733	1.00	20.21
1680	CZ	PHE	A	878	33.403	-11.138	11.660	1.00	20.82
1681	N	ASP	A	879	31.326	-9.268	6.973	1.00	19.57
1682	CA	ASP	A	879	31.800	-10.301	6.054	1.00	20.02
1683	C	ASP	A	879	32.723	-9.654	5.044	1.00	20.35
1684	O	ASP	A	879	33.802	-10.171	4.737	1.00	20.51
1685	CB	ASP	A	879	30.622	-10.972	5.342	1.00	20.24
1686	CG	ASP	A	879	29.693	-11.724	6.307	1.00	22.04
1687	OD1	ASP	A	879	30.122	-12.072	7.443	1.00	23.16
1688	OD2	ASP	A	879	28.520	-11.968	5.937	1.00	21.98
1689	N	LEU	A	880	32.342	-8.472	4.580	1.00	20.77
1690	CA	LEU	A	880	33.149	-7.775	3.596	1.00	20.33
1691	C	LEU	A	880	34.529	-7.496	4.136	1.00	20.40
1692	O	LEU	A	880	35.513	-7.723	3.453	1.00	21.41
1693	CB	LEU	A	880	32.484	-6.471	3.180	1.00	20.23
1694	CG	LEU	A	880	33.089	-5.838	1.939	1.00	18.50
1695	CD1	LEU	A	880	33.310	-6.886	0.855	1.00	19.38
1696	CD2	LEU	A	880	32.159	-4.762	1.477	1.00	18.07
1697	N	LEU	A	881	34.602	-7.040	5.376	1.00	20.90
1698	CA	LEU	A	881	35.882	-6.723	6.011	1.00	20.84
1699	C	LEU	A	881	36.818	-7.923	6.188	1.00	21.55
1700	O	LEU	A	881	38.055	-7.806	6.107	1.00	21.03
1701	CB	LEU	A	881	35.651	-6.055	7.364	1.00	19.23
1702	CG	LEU	A	881	36.989	-5.773	8.031	1.00	19.26
1703	CD1	LEU	A	881	37.662	-4.593	7.350	1.00	19.67
1704	CD2	LEU	A	881	36.810	-5.514	9.500	1.00	18.92

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1705	N	ILE	A	882	36.230	-9.063	6.492	1.00	22.39
	1706	CA	ILE	A	882	37.013	-10.265	6.671	1.00	23.63
	1707	C	ILE	A	882	37.668	-10.643	5.340	1.00	24.48
10	1708	O	ILE	A	882	38.859	-10.953	5.290	1.00	24.23
	1709	CB	ILE	A	882	36.136	-11.390	7.248	1.00	23.00
	1710	CG1	ILE	A	882	35.749	-11.006	8.675	1.00	22.91
15	1711 1	CG2	ILE	A	882	36.855	-12.729	7.185	1.00	22.75
	1712	CD1	ILE	A	882	36.922	-10.412	9.491	1.00	22.94
	1713	N	LYS	A	883	36.908	-10.541	4.256	1.00	25.73
20	1714	CA	LYS	A	883	37.441	-10.868	2.945	1.00	28.25
	1715	C	LYS	A	883	37.749	-9.657	2.061	1.00	30.08
	1716	O	LYS	A	883	37.823	-9.790	0.841	1.00	30.81
25	1717	CB	LYS	A	883	36.492	-11.820	2.211	1.00	27.47
	1718	CG	LYS	A	883	35.140	-11.240	1.932	1.00	27.17
	1719	CD	LYS	A	883	34.293	-12.163	1.109	1.00	27.60
30	1720	CE	LYS	A	883	32.926	-11.544	0.899	1.00	28.94
	1721	NZ	LYS	A	883	32.036	-12.319	-0.003	1.00	29.99
	1722	N	SER	A	884	37.976	-8.495	2.672	1.00	32.24
35	1723	CA	SER	A	884	38.268	-7.260	1.938	1.00	33.66
	1724	C	SER	A	884	39.500	-7.349	1.042	1.00	35.48
	1725	O	SER	A	884	39.491	-6.867	-0.087	1.00	35.08
40	1726	CB	SER	A	884	38.440	-6.106	2.921	1.00	32.96
	1727	OG	SER	A	884	39.466	-6.384	3.856	1.00	32.02
	1728	N	HIS	A	885	40.557	-7.969	1.556	1.00	38.15
45	1729	CA	HIS	A	885	41.815	-8.138	0.824	1.00	40.84
	1730	C	HIS	A	885	41.682	-9.017	-0.432	1.00	41.12
	1731	O	HIS	A	885	42.563	-9.010	-1.288	1.00	41.51
50	1732	CB	HIS	A	885	42.882	-8.688	1.789	1.00	43.70
	1733	CG	HIS	A	885	44.032	-9.392	1.124	1.00	47.44
	1734	ND1	HIS	A	885	45.172	-8.737	0.704	1.00	49.20
55	1735	CD2	HIS	A	885	44.240	-10.707	0.860	1.00	49.14
	1736	CE1	HIS	A	885	46.034	-9.615	0.217	1.00	49.74
	1737	NE2	HIS	A	885	45.493	-10.818	0.300	1.00	50.17
55	1738	N	MET	A	886	40.586	-9.762	-0.544	1.00	41.14
	1739	CA	MET	A	886	40.372	-10.639	-1.686	1.00	41.17
	1740	C	MET	A	886	39.455	-10.074	-2.761	1.00	40.68
	1741	O	MET	A	886	39.535	-10.476	-3.923	1.00	41.66

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1742	CB	MET	A	886	39.859	-11.989	-1.212	1.00	43.08
1743	CG	MET	A	886	40.928	-12.860	-0.584	1.00	45.59
1744	SD	MET	A	886	40.175	-14.113	0.457	1.00	50.78
1745	CE	MET	A	886	39.069	-14.971	-0.725	1.00	48.51
1746	N	VAL	A	887	38.542	-9.193	-2.370	1.00	39.25
1747	CA	VAL	A	887	37.637	-8.565	-3.333	1.00	37.55
1748	C	VAL	A	887	38.145	-7.168	-3.702	1.00	37.08
1749	O	VAL	A	887	37.484	-6.444	-4.442	1.00	37.26
1750	CB	VAL	A	887	36.187	-8.459	-2.802	1.00	37.19
1751	CG	VAL	A	887	35.526	-9.828	-2.756	1.00	37.49
1752	CG2	VAL	A	887	36.175	-7.817	-1.429	1.00	36.99
1753	N	SER	A	888	39.320	-6.809	-3.188	1.00	35.90
1754	CA	SER	A	888	39.955	-5.515	-3.437	1.00	35.05
1755	C	SER	A	888	39.216	-4.290	-2.898	1.00	34.27
1756	O	SER	A	888	39.402	-3.179	-3.396	1.00	34.78
1757	CB	SER	A	888	40.231	-5.342	-4.929	1.00	35.29
1758	OG	SER	A	888	41.335	-6.133	-5.326	1.00	36.74
1759	N	VAL	A	889	38.391	-4.485	-1.875	1.00	32.78
1760	CA	VAL	A	889	37.636	-3.386	-1.283	1.00	31.50
1761	C	VAL	A	889	38.410	-3.002	-0.064	1.00	31.36
1762	O	VAL	A	889	38.855	-3.895	0.648	1.00	32.20
1763	CB	VAL	A	889	36.244	-3.857	-0.772	1.00	30.79
1764	CG1	VAL	A	889	35.509	-2.729	-0.055	1.00	30.12
1765	CG2	VAL	A	889	35.410	-4.364	-1.903	1.00	30.08
1766	N	ASP	A	890	38.692	-1.724	0.156	1.00	31.10
1767	CA	ASP	A	890	39.364	-1.428	1.414	1.00	30.80
1768	C	ASP	A	890	38.629	-0.493	2.326	1.00	28.51
1769	O	ASP	A	890	37.889	0.379	1.889	1.00	27.96
1770	CB	ASP	A	890	40.849	-1.093	1.296	1.00	33.89
1771	CG	ASP	A	890	41.720	-1.949	2.261	1.00	35.96
1772	OD1	ASP	A	890	41.248	-2.314	3.373	1.00	35.86
1773	OD2	ASP	A	890	42.882	-2.260	1.901	1.00	37.33
1774	N	PHE	A	891	38.761	-0.782	3.610	1.00	26.20
1775	CA	PHE	A	891	38.096	-0.045	4.661	1.00	24.15
1776	C	PHE	A	891	39.036	0.942	5.305	1.00	24.58
1777	O	PHE	A	891	40.150	0.574	5.695	1.00	25.30
1778	CB	PHE	A	891	37.595	-1.027	5.732	1.00	20.51

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1779	CG	PHE	A	891	36.501	-1.937	5.259	1.00	16.33
	1780	CD1	PHE	A	891	36.741	-2.892	4.288	1.00	15.42
	1781	CD2	PHE	A	891	35.230	-1.826	5.773	1.00	14.37
10	1782	CE1	PHE	A	891	35.720	-3.730	3.832	1.00	13.60
	1783	CE2	PHE	A	891	34.220	-2.648	5.335	1.00	14.04
	1784	CZ	PHE	A	891	34.467	-3.607	4.353	1.00	13.43
15	1785	N	PRO	A	892	38.603	2.209	5.437	1.00	23.93
	1786	CA	PRO	A	892	39.441	3.234	6.060	1.00	23.41
	1787	C	PRO	A	892	39.655	2.866	7.520	1.00	23.31
20	1788	O	PRO	A	892	38.887	2.090	8.078	1.00	22.72
	1789	CB	PRO	A	892	38.582	4.485	5.940	1.00	23.21
	1790	CG	PRO	A	892	37.796	4.241	4.748	1.00	23.19
25	1791	CD	PRO	A	892	37.376	2.811	4.909	1.00	22.44
	1792	N	GLU	A	893	40.619	3.517	8.157	1.00	24.55
	1793	CA	GLU	A	893	40.984	3.267	9.555	1.00	26.50
30	1794	C	GLU	A	893	39.859	3.054	10.563	1.00	26.24
	1795	O	GLU	A	893	39.750	1.992	11.180	1.00	27.29
	1796	CB	GLU	A	893	41.885	4.385	10.072	1.00	28.90
35	1797	CG	GLU	A	893	42.329	4.192	11.509	1.00	33.98
	1798	CD	GLU	A	893	42.441	5.498	12.280	1.00	37.38
	1799	OE1	GLU	A	893	43.356	6.292	11.955	1.00	39.69
40	1800	OE2	GLU	A	893	41.624	5.729	13.216	1.00	39.34
	1801	N	MET	A	894	39.052	4.078	10.782	1.00	26.07
	1802	CA	MET	A	894	37.968	3.974	11.744	1.00	26.28
45	1803	C	MET	A	894	36.927	2.918	11.393	1.00	24.69
	1804	O	MET	A 894		36.337	2.311	12.287	1.00	24.64
	1805	CB	MET	A	894	37.313	5.337	11.954	1.00	28.30
50	1806	CG	MET	A	894	38.256	6.389	12.509	1.00	32.56
	1807	SD	MET	A	894	38.847	5.925	14.144	1.00	38.01
	1808	CE	MET	A	894	37.260	5.830	15.037	1.00	35.95
55	1809	N	MET	A 895		36.662	2.743	10.102	1.00	23.64
	1810	CA	MET	A	895	35.705	1.738	9.645	1.00	22.83
	1811	C	MET	A	895	36.171	0.328	10.032	1.00	22.26
60	1812	O	MET	A	895	35.469	-0.383	10.714	1.00	22.26
	1813	CB	MET	A	895	35.487	1.824	8.135	1.00	21.32
	1814	CG	MET	A	895	34.669	3.006	7.693	1.00	21.17
65	1815	SD	MET	A	895	33.044	3.064	8.432	1.00	20.56

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1816	CE	MET	A	895	32.088	2.305	7.205	1.00	22.81
	1817	N	ALA	A	896	37.362	-0.066	9.616	1.00	22.06
	1818	CA	ALA	A	896	37.867	-1.378	9.953	1.00	22.36
10	1819	C	ALA	A	896	37.914	-1.581	11.460	1.00	22.96
	1820	O	ALA	A	896	37.520	-2.630	11.947	1.00	23.87
	1821	CB	ALA	A	896	39.243	-1.588	9.350	1.00	22.56
15	1822	N	GLU	A	897	38.377	-0.586	12.212	1.00	23.92
	1823	CA	GLU	A	897	38.455	-0.724	13.666	1.00	24.05
	1824	C	GLU	A	897	37.076	-0.901	14.276	1.00	22.80
20	1825	O	GLU	A	897	36.873	-1.774	15.094	1.00	22.95
	1826	CB	GLU	A	897	39.128	0.502	14.313	1.00	25.98
	1827	CG	GLU	A	897	39.288	0.390	15.841	1.00	27.50
25	1828	CD	GLU	A	897	39.150	1.718	16.555	1.00	27.88
	1829	OE1	GLU	A	897	40.150	2.453	16.674	1.00	29.49
	1830	OE2	GLU	A	897	38.036	2.018	17.013	1.00	29.22
30	1831	N	ILE	A	898	36.129	-0.071	13.884	1.00	22.19
	1832	CA	ILE	A	898	34.801	-0.178	14.459	1.00	21.88
	1833	C	ILE	A	898	34.080	-1.398	13.968	1.00	20.49
35	1834	O	ILE	A	898	33.228	-1.917	14.656	1.00	21.90
	1835	CB	ILE	A	898	33.940	1.077	14.196	1.00	21.85
	1836	CG1	ILE	A	898	34.438	2.233	15.043	1.00	22.82
40	1837	CG2	ILE	A	898	32.478	0.836	14.587	1.00	22.66
	1838	CD1	ILE	A	898	33.490	3.390	15.019	1.00	23.11
	1839	N	ILE	A	899	34.410	-1.860	12.781	1.00	19.59
45	1840	CA	ILE	A	899	33.747	-3.027	12.248	1.00	19.42
	1841	C	ILE	A	899	34.305	-4.338	12.832	1.00	19.02
	1842	O	ILE	A	899	33.571	-5.300	12.982	1.00	19.98
50	1843	CB	ILE	A	899	33.758	-3.014	10.706	1.00	19.12
	1844	CG1	ILE	A	899	32.987	-1.786	10.187	1.00	18.56
	1845	CG2	ILE	A	899	33.095	-4.285	10.157	1.00	18.71
55	1846	CD1	ILE	A	899	33.054	-1.588	8.683	1.00	15.05
	1847	N	SER	A	900	35.565	-4.344	13.233	1.00	19.03
	1848	CA	SER	A	900	36.177	-5.518	13.822	1.00	19.74
	1849	C	SER	A	900	36.135	-5.502	15.355	1.00	20.48
	1850	O	SER	A	900	36.352	-6.521	16.010	1.00	21.19
	1851	CB	SER	A	900	37.614	-5.631	13.340	1.00	19.62
	1852	OG	SER	A	900	38.368	-4.478	13.683	1.00	22.08

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1853	N	VAL	A	901	35.866	-4.346	15.939	1.00	20.99
	1854	CA	VAL	A	901	35.808	-4.235	17.396	1.00	20.43
	1855	C	VAL	A	901	34.397	-4.087	17.935	1.00	20.42
10	1856	O	VAL	A	901	33.999	-4.823	18.841	1.00	21.68
	1857	CB	VAL	A	901	36.705	-3.074	17.927	1.00	20.22
	1858	CG1	VAL	A	901	36.407	-2.785	19.382	1.00	20.37
15	1859	CG2	VAL	A	901	38.168	-3.436	17.782	1.00	18.81
	1860	N	GLN	A	902	33.614	-3.187	17.350	1.00	19.34
	1861	CA	GLN	A	902	32.264	-2.957	17.828	1.00	17.55
20	1862	C	GLN	A	902	31.145	-3.766	17.207	1.00	16.24
	1863	O	GLN	A	902	30.337	-4.326	17.938	1.00	15.40
	1864	CB	GLN	A	902	31.929	-1.476	17.735	1.00	19.32
25	1865	CG	GLN	A	902	32.952	-0.579	18.371	1.00	20.82
	1866	CD	GLN	A	902	33.089	-0.776	19.861	1.00	23.15
	1867	OE1	GLN	A	902	32.211 1	-1.336	20.528	1.00	23.22
30	1868	NE2	GLN	A	902	34.197	-0.288	20.404	1.00	25.36
	1869	N	VAL	A	903	31.075	-3.810	15.872	1.00	15.79
	1870	CA	VAL	A	903	30.025	-4.552	15.144	1.00	15.22
35	1871	C	VAL	A	903	29.860	-6.010	15.605	1.00	14.74
	1872	O	VAL	A	903	28.732	-6.489	15.693	1.00	14.48
	1873	CB	VAL	A	903	30.195	-4.461	13.594	1.00	14.30
40	1874	CG1	VAL	A	903	29.159	-5.314	12.883	1.00	13.20
	1875	CG2	VAL	A	903	30.012	-3.005	13.147	1.00	14.90
	1876	N	PRO	A	904	30.976	-6.729	15.893	1.00	14.65
45	1877	CA	PRO	A	904	30.884	-8.122	16.356	1.00	15.80
	1878	C	PRO	A	904	30.053	-8.206	17.632	1.00	16.77
	1879	O	PRO	A	904	29.151	-9.039	17.713	1.00	18.38
50	1880	CB	PRO	A	904	32.350	-8.481	16.602	1.00	15.45
	1881	CG	PRO	A	904	33.014	-7.830	15.512	1.00	14.60
	1882	CD	PRO	A	904	32.377	-6.425	15.571	1.00	13.72
55	1883	N	LYS	A	905	30.286	-7.295	18.589	1.00	17.00
	1884	CA	LYS	A	905	29.525	-7.292	19.830	1.00	16.34
	1885	C	LYS	A	905	28.039	-7.273	19.546	1.00	15.58
55	1886	O	LYS	A	905	27.251	-7.817	20.297	1.00	15.43
	1887	CB	LYS	A	905	29.866	-6.085	20.668	1.00	18.17
	1888	CG	LYS	A	905	31.293	-6.007	21.132	1.00	19.96
	1889	CD	LYS	A	905	31.464	-4.733	21.947	1.00	22.09

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1890	CE	LYS	A	905	32.911	-4.429	22.276	1.00	23.59
1891	NZ	LYS	A	905	33.003	-3.173	23.083	1.00	27.13
1892	N	ILE	A	906	27.647	-6.620	18.466	1.00	15.71
1893	CA	ILE	A	906	26.239	-6.554	18.086	1.00	15.74
1894	C	ILE	A	906	25.800	-7.899	17.478	1.00	17.05
1895	O	ILE	A	906	24.759	-8.471	17.834	1.00	16.35
1896	CB	ILE	A	906	25.991	-5.423	17.030	1.00	14.76
1897	CG1	ILE	A	906	26.358	-4.051	17.611	1.00	13.40
1898	CG2	ILE	A	906	24.527	-5.427	16.565	1.00	13.47
1899	CD1	ILE	A	906	26.021	-2.876	16.686	1.00	13.18
1900	N	LEU	A	907	26.609	-8.385	16.539	1.00	17.95
1901	CA	LEU	A	907	26.348	-9.631	15.827	1.00	17.64
1902	C	LEU	A	907	26.386	-10.858	16.747	1.00	18.93
1903	O	LEU	A	907	25.756	-11.860	16.437	1.00	20.36
1904	CB	LEU	A	907	27.331	-9.787	14.659	1.00	15.32
1905	CG	LEU	A	907	27.338	-8.653	13.632	1.00	14.36
1906	CD1	LEU	A	907	28.382	-8.885	12.557	1.00	12.28
1907	CD2	LEU	A	907	25.947	-8.531	13.029	1.00	13.60
1908	N	SER	A	908	27.097	-10.805	17.868	1.00	19.02
1909	CA	SER	A	908	27.103	-11.947	18.772	1.00	19.60
1910	C	SER	A	908	26.027	-11.844	19.867	1.00	20.23
1911	O	SER	A	908	25.946	-12.709	20.752	1.00	20.86
1912	CB	SER	A	908	28.469	-12.099	19.407	1.00	19.21
1913	OG	SER	A	908	28.811	-10.944	20.135	1.00	19.20
1914	N	GLY	A	909	25.208	-10.791	19.812	1.00	19.30
1915	CA	GLY	A	909	24.169	-10.603	20.817	1.00	18.22
1916	C	GLY	A	909	24.533	-9.859	22.102	1.00	16.28
1917	O	GLY	A	909	23.711	-9.712	22.987	1.00	16.09
1918	N	LYS	A	910	25.773	-9.422	22.236	1.00	16.37
1919	CA	LYS	A	910	26.166	-8.670	23.411	1.00	17.37
1920	C	LYS	A	910	25.472	-7.296	23.532	1.00	18.68
1921	O	LYS	A	910	25.250	-6.797	24.640	1.00	19.51
1922	CB	LYS	A	910	27.665	-8.464	23.403	1.00	17.13
1923	CG	LYS	A	910	28.418	-9.703	23.684	1.00	16.32
1924	CD	LYS	A	910	29.860	-9.370	23.896	1.00	17.48
1925	CE	LYS	A	910	30.577	-10.534	24.482	1.00	17.90
1926	NZ	LYS	A	910	32.055	-10.284	24.502	1.00	19.93

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1927	N	VAL	A	911	25.219	-6.641	22.397	1.00	18.99
	1928	CA	VAL	A	911	24.545	-5.341	22.396	1.00	17.49
	1929	C	VAL	A	911	23.379	-5.475	21.458	1.00	17.48
10	1930	O	VAL	A	911	23.504	-6.015	20.358	1.00	17.40
	1931	CB	VAL	A	911	25.501	-4.130	22.041	1.00	17.52
	1932	CG1	VAL	A	911	26.928	-4.550	22.019	1.00	15.48
	1933	CG2	VAL	A	911	25.094	-3.412	20.788	1.00	15.48
15	1934	N	LYS	A	912	22.219	-5.032	21.896	1.00	17.96
	1935	CA	LYS	A	912	21.057	-5.210	21.072	1.00	19.32
	1936	C	LYS	A	912	20.262	-3.943	20.903	1.00	19.72
20	1937	O	LYS	A	912	20.437	-2.985	21.651	1.00	19.46
	1938	CB	LYS	A	912	20.189	-6.325	21.672	1.00	21.17
	1939	CG	LYS	A	912	19.261	-5.889	22.811	1.00	25.24
25	1940	CD	LYS	A	912	19.998	-5.297	24.030	1.00	26.63
	1941	CE	LYS	A	912	19.509	-3.871	24.370	1.00	26.56
	1942	NZ	LYS	A	912	18.028	-3.782	24.457	1.00	27.08
	1943	N	PRO	A	913	19.463	-3.877	19.841	1.00	20.13
30	1944	CA	PRO	A	913	18.693	-2.665	19.683	1.00	20.09
	1945	C	PRO	A	913	17.555	-2.665	20.658	1.00	20.77
	1946	O	PRO	A	913	17.108	-3.719	21.120	1.00	20.82
35	1947	CB	PRO	A	913	18.174	-2.780	18.259	1.00	20.97
	1948	CG	PRO	A	913	18.127	-4.240	18.017	1.00	21.02
	1949	CD	PRO	A	913	19.437	-4.660	18.599	1.00	20.38
	1950	N	ILE	A	914	17.094	-1.460	20.972	1.00	20.62
40	1951	CA	ILE	A	914	15.965	-1.262	21.846	1.00	18.90
	1952	C	ILE	A	914	14.823	-1.093	20.858	1.00	19.73
	1953	O	ILE	A	914	14.946	-0.313	19.909	1.00	20.71
45	1954	CB	ILE	A	914	16.119	0.012	22.659	1.00	17.34
	1955	CG1	ILE	A	914	17.445	-0.022	23.418	1.00	16.40
	1956	CG2	ILE	A	914	14.953	0.149	23.589	1.00	15.42
	1957	CD1	ILE	A	914	17.794	1.261	24.098	1.00	15.82
50	1958	N	TYR	A	915	13.774	-1.908	20.995	1.00	19.80
	1959	CA	TYR	A	915	12.622	-1.823	20.105	1.00	19.03
	1960	C	TYR	A	915	11.468	-1.273	20.882	1.00	18.68
55	1961	O	TYR	A	915	11.340	-1.494	22.080	1.00	18.72
	1962	CB	TYR	A	915	12.194	-3.193	19.566	1.00	18.88
	1963	CG	TYR	A	915	13.072	-3.773	18.505	1.00	18.76

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1964	CD1	TYR	A	915	14.096	-4.640	18.832	19.63
	1965	CD2	TYR	A	915	12.881	-3.457	17.173	19.64
	1966	CE1	TYR	A	915	14.923	-5.170	17.853	21.76
10	1967	CE2	TYR	A	915	13.698	-3.989	16.177	20.92
	1968	CZ	TYR	A	915	14.721	-4.839	16.531	21.98
	1969	OH	TYR	A	915	15.592	-5.314	15.577	25.00
	1970	N	PHE	A	916	10.621	-0.543	20.194	18.68
15	1971	CA	PHE	A	916	9.456	-0.019	20.836	19.66
	1972	C	PHE	A	916	8.451	-1.148	20.868	21.60
	1973	O	PHE	A	916	7.862	-1.434	21.910	22.04
20	1974	CB	PHE	A	916	8.898	1.145	20.042	17.07
	1975	CG	PHE	A	916	9.567	2.411	20.335	14.89
	1976	CD1	PHE	A	916	9.377	3.034	21.561	16.16
	1977	CD2	PHE	A	916	10.393	2.992	19.407	16.16
25	1978	CE1	PHE	A	916	10.010	4.225	21.854	14.78
	1979	CE2	PHE	A	916	11.028	4.183	19.689	16.01
	1980	CZ	PHE	A	916	10.836	4.800	20.916	15.28
30	1981	N	HIS	A	917	8.300	-1.804	19.718	22.86
	1982	CA	HIS	A	917	7.354	-2.899	19.543	24.45
	1983	C	HIS	A	917	8.077	-4.225	19.477	25.83
	1984	O	HIS	A	917	9.185	-4.257	18.908	27.53
35	1985	CB	HIS	A	917	6.549	-2.696	18.258	23.60
	1986	CG	HIS	A	917	5.921	-1.347	18.153	21.90
	1987	ND1	HIS	A	917	4.614	-1.109	18.504	21.41
40	1988	CD2	HIS	A	917	6.440	-0.153	17.787	21.97
	1989	CE1	HIS	A	917	4.350	0.178	18.360	22.05
	1990	NE2	HIS	A	917	5.446	0.783	17.929	21.26
	1991		HIS	A	917				
45	1992	C1	DHT		201	27.685	5.199	4.565	13.59
	1993	C2	DHT		201	26.814	6.485	4.636	12.55
	1994	C3	DHT		201	25.484	6.280	3.944	12.58
50	1995	O3	DHT		201	24.904	7.249	3.448	11.99
	1996	C4	DHT		201	24.887	4.964	3.857	13.18
	1997	C5	DHT		201	25.464	3.903	4.357	13.98
	1998	C6	DHT		201	24.727	2.560	4.241	14.79
55	1999	C7	DHT		201	25.613	1.454	3.609	14.79
	2000	C8	DHT		201	26.955	1.303	4.359	15.54

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TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2001	C9	DHT		201	27.708	2.656	4.279	1.00	14.37
2002	C10	DHT		201	26.943	3.876	4.949	1.00	14.56
2003	C11	DHT		201	29.161	2.525	4.830	1.00	14.73
2004	C12	DHT		201	29.951	1.344	4.192	1.00	14.11
2005	C13	DHT		201	29.194	-0.010	4.339	1.00	15.34
2006	C14	DHT		201	27.784	0.212	3.680	1.00	15.67
2007	C15	DHT		201	27.178	-1.232	3.647	1.00	15.64
2008	C16	DHT		201	28.435	-2.118	3.310	1.00	15.37
2009	C17	DHT		201	29.679	-1.189	3.426	1.00	14.87
2010	O17	DHT		201	30.910	-1.918	3.981	1.00	16.20
2011	C18	DHT		201	29.107	-0.450	5.847	1.00	14.67
2012	C19	DHT		201	26.781	3.770	6.524	1.00	13.94
2013	O	HOH		1	16.187	17.463	26.217	1.00	26.98
2014	O	HOH		2	19.878	17.183	14.290	1.00	13.49
2015	O	HOH		3	18.473	14.908	14.407	1.00	6.52
2016	O	HOH		4	29.144	18.703	11.673	1.00	37.40
2017	O	HOH		5	27.076	19.321	12.893	1.00	18.76
2018	O	HOH		6	23.789	12.817	9.649	1.00	33.78
2019	O	HOH		7	25.400	14.577	5.432	1.00	19.79
2020	O	HOH		8	23.015	12.473	12.245	1.00	14.03
2021	O	HOH		9	25.209	14.445	2.442	1.00	19.95
2022	O	HOH		10	34.235	16.490	0.235	1.00	41.09
2023	O	HOH		11	31.687	16.720	1.143	1.00	22.88
2024	O	HOH		12	26.451	12.094	2.237	1.00	8.25
2025	O	HOH		13	11.606	-0.191	-7.963	1.00	46.13
2026	O	HOH		14	13.798	0.894	17.657	1.00	15.30
2027	O	HOH		15	15.475	2.114	16.386	1.00	12.01
2028	O	HOH		16	8.514	-2.110	12.665	1.00	21.79
2029	O	HOH		17	23.094	0.783	14.094	1.00	10.94
2030	O	HOH		18	23.758	-13.306	5.541	1.00	40.43
2031	O	HOH		19	22.933	-11.472	10.611	1.00	31.03
2032	O	HOH		20	26.094	-11.914	5.354	1.00	51.71
2033	O	HOH		21	10.995	-6.843	16.294	1.00	29.91
2034	O	HOH		22	23.088	7.362	-10.811	1.00	30.10
2035	O	HOH		23	26.671	9.139	-8.686	1.00	38.12
2036	O	HOH		24	35.410	-8.438	-7.084	1.00	42.68
2037	O	HOH		25	10.842	24.253	21.391	1.00	43.09

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2038	O	HOH		26	40.376	-11.785	7.548	1.00	54.35
2039	O	HOH		27	1.671	16.382	5.866	1.00	24.50
2040	O	HOH		28	8.009	20.744	8.572	1.00	36.16
2041	O	HOH		29	29.490	17.190	30.961	1.00	56.26
2042	O	HOH		30	23.829	-12.134	25.596	1.00	39.41
2043	O	HOH		31	42.457	5.523	7.132	1.00	28.93
2044	O	HOH		32	41.318	2.323	2.406	1.00	38.22
2045	O	HOH		33	25.857	7.152	30.722	1.00	18.97
2046	O	HOH		34	18.191	16.505	27.701	1.00	29.01
2047	O	HOH		35	14.018	2.408	20.246	1.00	18.75
2048	O	HOH		36	14.651	4.006	17.873	1.00	21.70
2049	O	HOH		37	5.786	11.770	25.499	1.00	35.58
2050	O	HOH		38	30.734	13.383	-9.834	1.00	25.35
2051	O	HOH		39	0.334	6.151	20.624	1.00	27.66
2052	O	HOH		40	-2.677	2.639	17.420	1.00	35.67
2053	O	HOH		41	0.868	8.543	25.138	1.00	43.49
2054	O	HOH		42	-8.085	7.667	23.358	1.00	40.82
2055	O	HOH		43	6.749	1.200	9.766	1.00	24.57
2056	O	HOH		44	-0.636	8.734	6.585	1.00	40.09
2057	O	HOH		45	22.487	-4.734	14.335	1.00	28.04
2058	O	HOH		46	18.615	17.070	7.167	1.00	23.83
2059	O	HOH		47	38.089	13.268	-2.716	1.00	28.02
2060	O	HOH		48	29.251	-11.850	12.519	1.00	25.40
2061	O	HOH		49	23.684	9.361	5.898	1.00	24.06
2062	O	HOH		50	23.124	15.837	0.189	1.00	29.07
2063	O	HOH		51	34.079	8.287	19.446	1.00	34.35
2064	O	HOH		52	37.522	2.898	1.092	1.00	22.39
2065	O	HOH		53	21.838	14.392	5.445	1.00	20.42
2066	O	HOH		54	16.106	-10.859	0.784	1.00	48.09
2067	O	HOH		55	11.295	27.231	20.742	1.00	24.50
2068	O	HOH		56	21.562	-7.923	18.100	1.00	34.94
2069	O	HOH		57	41.647	-2.962	5.907	1.00	41.33
2070	O	HOH		58	12.897	22.682	24.938	1.00	44.10
2071	O	HOH		59	33.709	13.619	-5.931	1.00	26.84
2072	O	HOH		60	0.019	-4.834	14.164	1.00	36.91
2073	O	HOH		61	39.563	3.365	-2.334	1.00	36.56
2074	O	HOH		62	16.244	18.091	7.952	1.00	25.52

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2075	O	HOH		63	13.038	13.790	19.688	1.00	21.93
	2076	O	HOH		64	22.095	3.621	21.834	1.00	19.27
	2077	O	HOH		65	25.524	-2.235	39.160	1.00	30.91
10	2078	O	HOH		66	25.090	-1.064	36.971	1.00	31.16
	2079	O	HOH		67	5.186	-1.082	5.207	1.00	26.66
	2080	O	HOH		68	-0.310	15.229	24.529	1.00	28.42
15	2081	O	HOH		69	-6.181	9.210	18.935	1.00	37.84
	2082	O	HOH		70	17.508	26.662	14.814	1.00	30.32
	2083	O	HOH		71	17.401	31.211	13.007	1.00	30.57
20	2084	O	HOH		72	21.268	22.961	10.009	1.00	33.92
	2085	O	HOH		73	26.335	12.379	6.567	1.00	36.58
	2086	O	HOH		74	33.730	15.077	4.345	1.00	24.42
25	2087	O	HOH		75	28.576	2.290	-15.305	1.00	30.54
	2088	O	HOH		76	-5.886	5.402	21.276	1.00	48.01
	2089	O	HOH		77	31.878	-6.250	-10.283	1.00	38.45
30	2090	O	HOH		78	30.673	18.487	18.256	1.00	34.16
	2091	O	HOH		79	35.035	20.192	15.084	1.00	37.70
	2092	O	HOH		80	32.791	17.836	19.423	1.00	35.34
35	2093	O	HOH		81	22.587	-14.097	7.907	1.00	30.71
	2094	O	HOH		82	29.778	-9.620	-0.255	1.00	24.68
	2095	O	HOH		83	25.904	17.949	24.176	1.00	16.80
40	2096	O	HOH		84	33.066	-13.092	7.455	1.00	20.84
	2097	O	HOH		85	31.787	15.265	28.988	1.00	32.80
	2098	O	HOH		86	27.029	0.835	13.994	1.00	20.01
45	2099	O	HOH		87	20.499	2.720	16.384	1.00	31.66
	2100	O	HOH		88	10.991	16.858	-1.085	1.00	30.58
	2101	O	HOH		89	7.904	10.344	-5.081	1.00	41.55
50	2102	O	HOH		90	12.570	3.398	-10.099	1.00	26.95
	2103	O	HOH		91	17.128	3.214	-10.962	1.00	22.24
	2104	O	HOH		92	17.056	1.547	-4.553	1.00	26.98
55	2105	O	HOH		93	11.020	0.892	6.595	1.00	25.24
	2106	O	HOH		94	24.948	1.135	35.230	1.00	27.44
	2107	O	HOH		95	24.006	5.653	35.765	1.00	34.54
55	2108	O	HOH		96	29.738	0.950	27.680	1.00	26.47
	2109	O	HOH		97	1.507	8.706	22.315	1.00	36.26
	2110	O	HOH		98	10.755	-4.751	9.776	1.00	27.77
	2111	O	HOH		99	20.223	-3.560	14.440	1.00	25.10

TABLE 8 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH DHT									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2112	O	HOH		100	30.147	-9.103	2.467	1.00	26.08
2113	O	HOH		101	28.518	-12.565	-5.152	1.00	28.96
2114	O	HOH		102	39.044	7.751	17.961	1.00	38.02
2115	O	HOH		103	37.030	10.428	20.994	1.00	37.73
2116	O	HOH		104	7.847	-2.227	15.270	1.00	24.79
2117	O	HOH		105	9.958	-5.351	21.522	1.00	40.62
2118	O	HOH		106	21.201	6.928	-12.688	1.00	30.96

TABLE 9

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1	N	CYS	A	669	22.921	9.448	24.884	1.00	77.12
2	CA	CYS	A	669	22.859	9.723	23.414	1.00	86.87
3	C	CYS	A	669	21.892	8.793	22.633	1.00	86.11
4	O	CYS	A	669	22.074	8.565	21.427	1.00	77.81
5	CB	CYS	A	669	24.276	9.675	22.802	1.00	88.59
6	SG	CYS	A	669	24.838	11.217	21.992	1.00	94.18
7	N	GLN	A	670	20.835	8.318	23.308	1.00	87.01
8	CA	GLN	A	670	19.841	7.405	22.705	1.00	89.27
9	C	GLN	A	670	18.731	8.155	21.935	1.00	86.82
10	O	GLN	A	670	18.184	9.157	22.427	1.00	85.28
11	CB	GLN	A	670	19.222	6.498	23.792	1.00	93.96
12	CG	GLN	A	670	18.335	5.330	23.282	1.00	90.90
13	CD	GLN	A	670	18.946	3.972	23.548	1.00	89.73
14	OE1	GLN	A	670	19.840	3.532	22.833	1.00	86.20
15	NE2	GLN	A	670	18.456	3.297	24.575	1.00	91.02
16	N	PRO	A	671	18.312	7.612	20.764	1.00	82.62
17	CA	PRO	A	671	17.273	8.224	19.921	1.00	76.72
18	C	PRO	A	671	15.795	8.270	20.367	1.00	71.10
19	O	PRO	A	671	14.933	8.452	19.508	1.00	75.36
20	CB	PRO	A	671	17.414	7.449	18.599	1.00	73.17
21	CG	PRO	A	671	17.777	6.058	19.076	1.00	75.93
22	CD	PRO	A	671	18.835	6.381	20.127	1.00	80.30
23	N	ILE	A	672	15.473	8.187	21.661	1.00	59.44
24	CA	ILE	A	672	14.045	8.210	22.043	1.00	57.16
25	C	ILE	A	672	13.232	9.465	21.682	1.00	59.85
26	O	ILE	A	672	12.069	9.358	21.234	1.00	54.31

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	27	CB	ILE	A	672	13.792	7.852	23.525	1.00	54.74
	28	CG1	ILE	A	672	12.353	8.234	23.892	1.00	47.09
	29	CG2	ILE	A	672	14.835	8.496	24.426	1.00	64.17
10	30	CD1	ILE	A	672	11.963	7.922	25.277	1.00	56.37
	31	N	PHE	A	673	13.834	10.642	21.885	1.00	61.01
	32	CA	PHE	A	673	13.167	11.909	21.583	1.00	53.54
15	33	C	PHE	A	673	12.960	12.039	20.068	1.00	44.47
	34	O	PHE	A	673	11.858	12.376	19.585	1.00	38.12
	35	CB	PHE	A	673	13.980	13.095	22.129	1.00	55.20
20	36	CG	PHE	A	673	13.247	14.403	22.055	1.00	54.87
	37	CD1	PHE	A	673	12.248	14.703	22.976	1.00	54.05
	38	CD2	PHE	A	673	13.491	15.292	21.017	1.00	47.32
25	39	CE1	PHE	A	673	11.500	15.858	22.860	1.00	53.41
	40	CE2	PHE	A	673	12.749	16.448	20.897	1.00	49.17
	41	CZ	PHE	A	673	11.749	16.730	21.816	1.00	53.29
30	42	N	LEU	A	674	14.023	11.743	19.327	1.00	36.26
	43	CA	LEU	A	674	13.976	11.789	17.882	1.00	38.85
	44	C	LEU	A	674	12.919	10.866	17.273	1.00	38.35
35	45	O	LEU	A	674	12.254	11.238	16.300	1.00	39.82
	46	CB	LEU	A	674	15.358	11.487	17.303	1.00	45.56
	47	CG	LEU	A	674	16.279	12.708	17.252	1.00	49.73
40	48	CD1	LEU	A	674	17.687	12.339	16.760	1.00	48.00
	49	CD2	LEU	A	674	15.638	13.737	16.318	1.00	42.53
	50	N	ASN	A	675	12.731	9.686	17.871	1.00	40.82
45	51	CA	ASN	A	675	11.744	8.705	17.370	1.00	41.39
	52	C	ASN	A	675	10.374	9.297	17.456	1.00	39.61
	53	O	ASN	A	675	9.527	9.092	16.568	1.00	33.60
50	54	CB	ASN	A	675	11.734	7.434	18.209	1.00	51.05
	55	CG	ASN	A	675	13.008	6.648	18.091	1.00	55.02
	56	OD1	ASN	A	675	13.672	6.651	17.045	1.00	54.01
55	57	ND2	ASN	A	675	13.370	5.971	19.166	1.00	60.08
	58	N	VAL	A	676	10.159	10.022	18.551	1.00	37.88
	59	CA	VAL	A	676	8.894	10.687	18.781	1.00	36.37
55	60	C	VAL	A	676	8.669	11.777	17.736	1.00	39.08
	61	O	VAL	A	676	7.631	11.798	17.072	1.00	43.18
	62	CB	VAL	A	676	8.821	11.336	20.153	1.00	36.30
	63	CG1	VAL	A	676	7.421	11.860	20.358	1.00	29.55

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	64	CG2	VAL	A	676	9.187	10.341	21.236	1.00	30.15
	65	N	LEU	A	677	9.637	12.667	17.547	1.00	38.08
	66	CA	LEU	A	677	9.429	13.726	16.565	1.00	37.80
10	67	C	LEU	A	677	9.188	13.208	15.156	1.00	38.78
	68	O	LEU	A	677	8.324	13.730	14.448	1.00	44.11
	69	CB	LEU	A	677	10.571	14.726	16.574	1.00	34.97
15	70	CG	LEU	A	677	10.812	15.352	17.943	1.00	40.42
	71	CD1	LEU	A	677	11.862	16.404	17.760	1.00	35.87
	72	CD2	LEU	A	677	9.511	15.944	18.534	1.00	39.49
20	73	N	GLU	A	678	9.927	12.170	14.764	1.00	34.27
	74	CA	GLU	A	678	9.788	11.576	13.433	1.00	33.68
	75	C	GLU	A	678	8.502	10.791	13.361	1.00	31.24
25	76	O	GLU	A	678	7.837	10.730	12.318	1.00	29.04
	77	CB	GLU	A	678	10.972	10.692	13.139	1.00	41.54
	78	CG	GLU	A	678	12.250	11.475	13.231	1.00	62.50
30	79	CD	GLU	A	678	13.492	10.632	13.140	1.00	75.90
	80	OE1	GLU	A	678	13.382	9.393	13.275	1.00	81.73
	81	OE2	GLU	A	678	14.581	11.222	12.946	1.00	77.79
35	82	N	ALA	A	679	8.118	10.229	14.496	1.00	27.29
	83	CA	ALA	A	679	6.878	9.486	14.561	1.00	31.51
	84	C	ALA	A	679	5.658	10.400	14.416	1.00	37.88
40	85	O	ALA	A	679	4.657	10.013	13.784	1.00	39.80
	86	CB	ALA	A	679	6.807	8.699	15.862	1.00	32.16
	87	N	ILE	A	680	5.748	11.621	14.958	1.00	36.75
45	88	CA	ILE	A	680	4.623	12.567	14.893	1.00	33.51
	89	C	ILE	A	680	4.603	13.553	13.732	1.00	29.78
	90	O	ILE	A	680	3.560	14.137	13.425	1.00	35.01
50	91	CB	ILE	A	680	4.445	13.322	16.204	1.00	36.86
	92	CG1	ILE	A	680	5.672	14.178	16.493	1.00	39.01
	93	CG2	ILE	A	680	4.222	12.324	17.343	1.00	34.87
55	94	CD1	ILE	A	680	5.503	15.046	17.719	1.00	38.54
	95	N	GLU	A	681	5.732	13.677	13.044	1.00	31.29
	96	CA	GLU	A	681	5.833	14.570	11.904	1.00	36.50
55	97	C	GLU	A	681	4.638	14.373	11.013	1.00	38.74
	98	O	GLU	A	681	4.348	13.251	10.596	1.00	46.06
	99	CB	GLU	A	681	7.101	14.285	11.106	1.00	33.49
	100	CG	GLU	A	681	7.361	15.322	10.028	1.00	41.42

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	101	CD	GLU	A	681	7.500	16.742	10.581	49.46
	102	OE1	GLU	A	681	7.569	16.924	11.824	44.22
	103	OE2	GLU	A	681	7.527	17.687	9.759	52.12
10	104	N	PRO	A	682	3.892	15.446	10.751	41.06
	105	CA	PRO	A	682	2.695	15.422	9.904	41.12
	106	C	PRO	A	682	2.968	14.980	8.444	44.28
	107	O	PRO	A	682	4.076	15.133	7.920	36.92
15	108	CB	PRO	A	682	2.214	16.870	9.965	43.30
	109	CG	PRO	A	682	2.800	17.399	11.250	38.89
	110	CD	PRO	A	682	4.159	16.800	11.261	39.59
20	111	N	GLY	A	683	1.943	14.446	7.788	48.21
	112	CA	GLY	A	683	2.103	13.990	6.416	51.13
	113	C	GLY	A	683	1.905	15.043	5.334	54.68
	114	O	GLY	A	683	1.817	16.226	5.629	63.53
25	115	N	VAL	A	684	1.729	14.601	4.089	57.20
	116	CA	VAL	A	684	1.544	15.505	2.959	54.91
	117	C	VAL	A	684	0.123	16.048	2.952	54.45
30	118	O	VAL	A	684	-0.828	15.287	2.775	57.51
	119	CB	VAL	A	684	1.805	14.792	1.625	51.72
	120	CG1	VAL	A	684	1.618	15.769	0.487	53.17
	121	CG2	VAL	A	684	3.222	14.212	1.591	53.92
35	122	N	VAL	A	685	-0.021	17.360	3.125	48.43
	123	CA	VAL	A	685	-1.341	17.974	3.163	44.96
	124	C	VAL	A	685	-1.603	18.758	1.887	46.69
40	125	O	VAL	A	685	-0.934	19.742	1.644	54.09
	126	CB	VAL	A	685	-1.455	18.932	4.355	39.06
	127	CG1	VAL	A	685	-2.888	19.062	4.764	41.14
	128	CG2	VAL	A	685	-0.611	18.445	5.520	36.12
45	129	N	CYS	A	686	-2.582	18.340	1.087	51.49
	130	CA	CYS	A	686	-2.921	19.015	-0.177	55.13
	131	C	CYS	A	686	-3.830	20.266	-0.010	56.12
50	132	O	CYS	A	686	-4.856	20.208	0.681	54.29
	133	CB	CYS	A	686	-3.559	18.009	-1.155	57.05
	134	SG	CYS	A	686	-2.391	16.910	-2.025	65.52
55	135	N	ALA	A	687	-3.484	21.374	-0.681	54.36
	136	CA	ALA	A	687	-4.248	22.631	-0.584	54.20
	137	C	ALA	A	687	-5.583	22.542	-1.268	60.58

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
138	O	ALA	A	687	-6.557	23.131	-0.803	1.00	62.87
139	CB	ALA	A	687	-3.463	23.815	-1.168	1.00	49.21
140	N	GLY	A	688	-5.623	21.791	-2.366	1.00	67.12
141	CA	GLY	A	688	-6.847	21.650	-3.134	1.00	66.26
142	C	GLY	A	688	-6.948	22.874	-4.024	1.00	64.95
143	O	GLY	A	688	-7.888	23.676	-3.924	1.00	66.95
144	N	HIS	A	689	-5.951	23.042	-4.879	1.00	59.22
145	CA	HIS	A	689	-5.925	24.179	-5.769	1.00	54.36
146	C	HIS	A	689	-6.022	23.716	-7.220	1.00	59.75
147	O	HIS	A	689	-5.393	22.717	-7.602	1.00	62.11
148	CB	HIS	A	689	-4.650	24.977	-5.537	1.00	46.90
149	CG	HIS	A	689	-4.364	25.964	-6.617	1.00	52.16
150	ND1	HIS	A	689	-5.104	27.116	-6.787	1.00	52.66
151	CD2	HIS	A	689	-3.474	25.931	-7.633	1.00	58.89
152	CE1	HIS	A	689	-4.683	27.750	-7.868	1.00	57.16
153	NE2	HIS	A	689	-3.695	27.052	-8.402	1.00	60.29
154	N	ASP	A	690	-6.838	24.424	-8.011	1.00	60.46
155	CA	ASP	A	690	-7.021	24.108	-9.427	1.00	59.31
156	C	ASP	A	690	-5.835	24.583	-10.280	1.00	60.15
157	O	ASP	A	690	-5.739	25.752	-10.654	1.00	58.71
158	CB	ASP	A	690	-8.334	24.701	-9.949	1.00	60.31
159	CG	ASP	A	690	-8.762	24.107	-11.304	1.00	62.54
160	OD1	ASP	A	690	-7.904	23.586	-12.054	1.00	54.14
161	OD2	ASP	A	690	-9.970	24.166	-11.620	1.00	59.85
162	N	ASN	A	691	-4.925	23.657	-10.564	1.00	66.30
163	CA	ASN	A	691	-3.736	23.940	-11.369	1.00	71.61
164	C	ASN	A	691	-4.037	23.857	-12.868	1.00	73.70
165	O	ASN	A	691	-3.121	23.715	-13.682	1.00	81.27
166	CB	ASN	A	691	-2.581	22.971	-11.016	1.00	72.66
167	CG	ASN	A	691	-1.672	23.506	-9.923	1.00	72.16
168	OD1	ASN	A	691	-1.697	24.697	-9.600	1.00	74.90
169	ND2	ASN	A	691	-0.845	22.633	-9.365	1.00	72.55
170	N	ASN	A	692	-5.317	23.908	-13.227	1.00	70.75
171	CA	ASN	A	692	-5.705	23.851	-14.632	1.00	69.77
172	C	ASN	A	692	-6.467	25.131	-14.982	1.00	66.04
173	O	ASN	A	692	-6.986	25.257	-16.087	1.00	65.61
174	CB	ASN	A	692	-6.551	22.600	-14.958	1.00	68.43

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	175	CG	ASN	A	692	-6.019	21.331	-14.307	1.00	63.97
	176	OD1	ASN	A	692	-5.501	20.438	-14.972	0.00	65.30
	177	ND2	ASN	A	692	-6.184	21.240	-12.993	0.00	65.24
10	178	N	GLN	A	693	-6.597	26.035	-14.005	1.00	67.69
	179	CA	GLN	A	693	-7.255	27.340	-14.196	1.00	71.99
	180	C	GLN	A	693	-6.171	28.429	-14.199	1.00	74.61
15	181	O	GLN	A	693	-5.230	28.359	-13.413	1.00	73.58
	182	CB	GLN	A	693	-8.279	27.647	-13.084	1.00	68.47
	183	CG	GLN	A	693	-9.575	26.819	-13.134	1.00	72.04
20	184	CD	GLN	A	693	-10.172	26.661	-14.540	1.00	75.91
	185	OE1	GLN	A	693	-9.955	27.497	-15.423	1.00	85.37
	186	NE2	GLN	A	693	-10.936	25.592	-14.745	1.00	70.58
25	187	N	PRO	A	694	-6.285	29.438	-15.091	1.00	81.70
	188	CA	PRO	A	694	-5.302	30.531	-15.181	1.00	80.62
	189	C	PRO	A	694	-5.118	31.249	-13.856	1.00	77.25
30	190	O	PRO	A	694	-6.106	31.640	-13.206	1.00	74.33
	191	CB	PRO	A	694	-5.911	31.458	-16.243	1.00	85.84
	192	CG	PRO	A	694	-7.421	31.170	-16.151	1.00	89.04
35	193	CD	PRO	A	694	-7.398	29.662	-16.034	1.00	87.17
	194	N	ASP	A	695	-3.849	31.467	-13.496	1.00	76.00
	195	CA	ASP	A	695	-3.494	32.117	-12.237	1.00	63.22
40	196	C	ASP	A	695	-4.294	33.356	-11.942	1.00	56.02
	197	O	ASP	A	695	-4.859	33.997	-12.842	1.00	56.35
	198	CB	ASP	A	695	-1.995	32.405	-12.153	1.00	63.70
45	199	CG	ASP	A	695	-1.190	31.192	-11.684	1.00	66.50
	200	OD1	ASP	A	695	-1.523	30.627	-10.617	1.00	66.69
	201	OD2	ASP	A	695	-0.217	30.802	-12.377	1.00	71.13
50	202	N	SER	A	696	-4.338	33.694	-10.666	1.00	56.40
	203	CA	SER	A	696	-5.093	34.839	-10.214	1.00	56.56
	204	C	SER	A	696	-4.690	35.191	-8.788	1.00	61.68
55	205	O	SER	A	696	-4.326	34.319	-7.993	1.00	69.36
	206	CB	SER	A	696	-6.587	34.510	-10.289	1.00	54.32
	207	OG	SER	A	696	-7.365	35.473	-9.604	1.00	54.41
	208	N	PHE	A	697	-4.754	36.477	-8.474	1.00	61.93
	209	CA	PHE	A	697	-4.412	36.974	-7.153	1.00	61.05
	210	C	PHE	A	697	-5.344	36.448	-6.037	1.00	61.34
	211	O	PHE	A	697	-4.881	36.053	-4.971	1.00	62.55

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
212	CB	PHE	A	697	-4.413	38.509	-7.195	1.00	63.27
213	CG	PHE	A	697	-4.961	39.156	-5.951	1.00	60.53
214	CD1	PHE	A	697	-4.142	39.397	-4.856	1.00	65.55
215	CD2	PHE	A	697	-6.306	39.484	-5.864	1.00	61.74
216	CE1	PHE	A	697	-4.651	39.950	-3.691	1.00	63.81
217	CE2	PHE	A	697	-6.825	40.034	-4.710	1.00	66.91
218	CZ	PHE	A	697	-5.994	40.267	-3.617	1.00	69.41
219	N	ALA	A	698	-6.653	36.464	-6.261	1.00	58.96
220	CA	ALA	A	698	-7.577	35.996	-5.230	1.00	59.58
221	C	ALA	A	698	-7.653	34.467	-5.143	1.00	61.20
222	O	ALA	A	698	-7.862	33.913	-4.063	1.00	64.62
223	CB	ALA	A	698	-8.965	36.589	-5.448	1.00	56.65
224	N	ALA	A	699	-7.492	33.783	-6.272	1.00	58.65
225	CA	ALA	A	699	-7.555	32.328	-6.270	1.00	57.39
226	C	ALA	A	699	-6.290	31.748	-5.616	1.00	54.55
227	O	ALA	A	699	-6.349	30.708	-4.951	1.00	57.04
228	CB	ALA	A	699	-7.749	31.791	-7.694	1.00	58.30
229	N	LEU	A	700	-5.155	32.423	-5.786	1.00	44.77
230	CA	LEU	A	700	-3.921	31.956	-5.181	1.00	40.04
231	C	LEU	A	700	-3.983	32.180	-3.667	1.00	40.02
232	O	LEU	A	700	-3.737	31.256	-2.893	1.00	42.09
233	CB	LEU	A	700	-2.709	32.661	-5.800	1.00	40.84
234	CG	LEU	A	700	-2.369	32.286	-7.251	1.00	47.93
235	CD1	LEU	A	700	-1.195	33.092	-7.751	1.00	52.49
236	CD2	LEU	A	700	-2.035	30.824	-7.337	1.00	41.70
237	N	LEU	A	701	-4.384	33.375	-3.238	1.00	38.79
238	CA	LEU	A	701	-4.468	33.679	-1.808	1.00	40.37
239	C	LEU	A	701	-5.548	32.917	-1.024	1.00	45.30
240	O	LEU	A	701	-5.305	32.557	0.128	1.00	45.13
241	CB	LEU	A	701	-4.545	35.190	-1.561	1.00	37.85
242	CG	LEU	A	701	-3.253	35.971	-1.868	1.00	41.30
243	CD1	LEU	A	701	-3.479	37.426	-1.612	1.00	41.50
244	CD2	LEU	A	701	-2.070	35.506	-1.025	1.00	35.31
245	N	SER	A	702	-6.719	32.678	-1.633	1.00	52.36
246	CA	SER	A	702	-7.822	31.899	-1.013	1.00	54.37
247	C	SER	A	702	-7.388	30.433	-0.783	1.00	51.62
248	O	SER	A	702	-7.740	29.806	0.234	1.00	45.03

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
249	CB	SER	A	702	-9.060	31.920	-1.914	1.00	50.95
250	OG	SER	A	702	-9.500	33.246	-2.101	1.00	50.66
251	N	SER	A	703	-6.649	29.890	-1.756	1.00	49.24
252	CA	SER	A	703	-6.119	28.536	-1.660	1.00	46.51
253	C	SER	A	703	-5.101	28.504	-0.528	1.00	46.34
254	O	SER	A	703	-5.141	27.597	0.293	1.00	52.79
255	CB	SER	A	703	-5.442	28.115	-2.956	1.00	37.23
256	OG	SER	A	703	-6.388	28.080	-4.005	1.00	45.32
257	N	LEU	A	704	-4.215	29.501	-0.459	1.00	40.74
258	CA	LEU	A	704	-3.227	29.548	0.618	1.00	36.98
259	C	LEU	A	704	-3.902	29.552	1.984	1.00	41.66
260	O	LEU	A	704	-3.389	28.951	2.920	1.00	45.02
261	CB	LEU	A	704	-2.302	30.751	0.485	1.00	30.44
262	CG	LEU	A	704	-0.994	30.563	-0.291	1.00	35.89
263	CD1	LEU	A	704	-0.235	31.859	-0.308	1.00	36.89
264	CD2	LEU	A	704	-0.115	29.484	0.307	1.00	37.91
265	N	ASN	A	705	-5.061	30.208	2.076	1.00	45.16
266	CA	ASN	A	705	-5.849	30.289	3.311	1.00	43.35
267	C	ASN	A	705	-6.521	28.962	3.618	1.00	42.54
268	O	ASN	A	705	-6.677	28.594	4.779	1.00	40.34
269	CB	ASN	A	705	-6.934	31.370	3.201	1.00	44.83
270	CG	ASN	A	705	-6.362	32.771	3.137	1.00	43.71
271	OD1	ASN	A	705	-5.197	32.992	3.470	1.00	48.81
272	ND2	ASN	A	705	-7.176	33.726	2.694	1.00	38.59
273	N	GLU	A	706	-6.991	28.269	2.591	1.00	42.62
274	CA	GLU	A	706	-7.607	26.987	2.842	1.00	44.02
275	C	GLU	A	706	-6.478	26.033	3.261	1.00	42.46
276	O	GLU	A	706	-6.639	25.253	4.195	1.00	42.70
277	CB	GLU	A	706	-8.352	26.472	1.621	1.00	45.19
278	CG	GLU	A	706	-9.322	25.338	1.971	1.00	55.97
279	CD	GLU	A	706	-10.417	25.735	2.986	1.00	58.77
280	OE1	GLU	A	706	-11.019	26.817	2.838	1.00	60.87
281	OE2	GLU	A	706	-10.707	24.945	3.918	1.00	60.16
282	N	LEU	A	707	-5.307	26.167	2.636	1.00	38.31
283	CA	LEU	A	707	-4.152	25.342	2.982	1.00	37.96
284	C	LEU	A	707	-3.767	25.654	4.431	1.00	44.27
285	O	LEU	A	707	-3.464	24.747	5.211	1.00	51.41

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	286	CB	LEU	A	707	-2.958	25.608	2.046	1.00	35.41
	287	CG	LEU	A	707	-1.651	24.872	2.392	1.00	35.71
	288	CD1	LEU	A	707	-1.895	23.385	2.326	1.00	38.82
10	289	CD2	LEU	A	707	-0.518	25.239	1.459	1.00	33.25
	290	N	GLY	A	708	-3.782	26.938	4.787	1.00	45.88
	291	CA	GLY	A	708	-3.463	27.344	6.144	1.00	40.92
15	292	C	GLY	A	708	-4.386	26.618	7.096	1.00	39.05
	293	O	GLY	A	708	-3.937	25.851	7.924	1.00	45.81
	294	N	GLU	A	709	-5.685	26.790	6.913	1.00	46.04
20	295	CA	GLU	A	709	-6.680	26.125	7.758	1.00	51.25
	296	C	GLU	A	709	-6.367	24.637	7.975	1.00	51.93
	297	O	GLU	A	709	-6.213	24.197	9.107	1.00	56.39
25	298	CB	GLU	A	709	-8.079	26.273	7.151	1.00	56.56
	299	CG	GLU	A	709	-9.198	25.652	7.984	1.00	63.02
	300	CD	GLU	A	709	-9.766	26.593	9.042	1.00	64.61
30	301	OE1	GLU	A	709	-9.157	27.641	9.338	1.00	66.14
	302	OE2	GLU	A	709	-10.855	26.293	9.573	1.00	65.41
	303	N	ARG	A	710	-6.235	23.864	6.901	1.00	53.43
35	304	CA	ARG	A	710	-5.938	22.440	7.058	1.00	50.19
	305	C	ARG	A	710	-4.617	22.102	7.735	1.00	44.91
	306	O	ARG	A	710	-4.522	21.061	8.396	1.00	43.38
40	307	CB	ARG	A	710	-6.032	21.652	5.747	1.00	56.69
	308	CG	ARG	A	710	-6.192	22.446	4.493	1.00	59.66
	309	CD	ARG	A	710	-7.462	22.035	3.786	1.00	59.37
45	310	NE	ARG	A	710	-7.203	21.172	2.643	1.00	58.69
	311	CZ	ARG	A	710	-8.124	20.857	1.736	1.00	70.01
	312	NH1	ARG	A	710	-9.364	21.349	1.854	1.00	75.20
50	313	NH2	ARG	A	710	-7.812	20.057	0.713	1.00	65.26
	314	N	GLN	A	711	-3.596	22.939	7.556	1.00	40.11
	315	CA	GLN	A	711	-2.310	22.685	8.189	1.00	34.69
55	316	C	GLN	A	711	-2.355	23.007	9.653	1.00	36.60
	317	O	GLN	A	711	-1.501	22.557	10.408	1.00	40.79
	318	CB	GLN	A	711	-1.194	23.478	7.542	1.00	42.15
55	319	CG	GLN	A	711	-0.753	22.877	6.244	1.00	43.03
	320	CD	GLN	A	711 1	0.553	23.442	5.779	1.00	44.24
	321	OE1	GLN	A	711	1.321	23.988	6.567	1.00	54.32
	322	NE2	GLN	A	711	0.828	23.305	4.496	1.00	52.33

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
323	N	LEU	A	712	-3.361	23.778	10.054	1.00	41.25
324	CA	LEU	A	712	-3.561	24.163	11.457	1.00	43.47
325	C	LEU	A	712	-4.061	22.938	12.222	1.00	45.20
326	O	LEU	A	712	-3.595	22.628	13.320	1.00	46.51
327	CB	LEU	A	712	-4.585	25.295	11.550	1.00	42.08
328	CG	LEU	A	712	-4.829	25.943	12.905	1.00	45.04
329	CD1	LEU	A	712	-3.489	26.199	13.594	1.00	48.18
330	CD2	LEU	A	712	-5.610	27.248	12.711	1.00	44.32
331	N	VAL	A	713	-5.014	22.240	11.623	1.00	42.76
332	CA	VAL	A	713	-5.555	21.026	12.198	1.00	41.99
333	C	VAL	A	713	-4.383	20.100	12.562	1.00	45.10
334	O	VAL	A	713	-4.275	19.646	13.703	1.00	45.64
335	CB	VAL	A	713	-6.480	20.348	11.170	1.00	43.85
336	CG1	VAL	A	713	-6.887	18.953	11.628	1.00	52.59
337	CG2	VAL	A	713	-7.708	21.203	10.966	1.00	42.38
338	N	HIS	A	714	-3.471	19.905	11.604	1.00	46.35
339	CA	HIS	A	714	-2.286	19.044	11.767	1.00	45.95
340	C	HIS	A	714	-1.379	19.495	12.857	1.00	43.82
341	O	HIS	A	714	-0.798	18.674	13.571	1.00	48.61
342	CB	HIS	A	714	-1.458	18.971	10.487	1.00	49.61
343	CG	HIS	A	714	-1.950	17.947	9.519	1.00	62.09
344	ND1	HIS	A	714	-3.157	18.058	8.873	1.00	63.02
345	CD2	HIS	A	714	-1.404	16.778	9.108	1.00	64.82
346	CE1	HIS	A	714	-3.340	17.005	8.100	1.00	70.96
347	NE2	HIS	A	714	-2.291	16.211	8.219	1.00	70.54
348	N	VAL	A	715	-1.172	20.803	12.898	1.00	40.29
349	CA	VAL	A	715	-0.326	21.415	13.908	1.00	39.63
350	C	VAL	A	715	-0.962	21.201	15.273	1.00	36.62
351	O	VAL	A	715	-0.266	20.874	16.244	1.00	30.18
352	CB	VAL	A	715	-0.101	22.918	13.620	1.00	38.77
353	CG1	VAL	A	715	0.500	23.617	14.820	1.00	30.17
354	CG2	VAL	A	715	0.857	23.048	12.463	1.00	40.69
355	N	VAL	A	716	-2.286	21.329	15.331	1.00	28.64
356	CA	VAL	A	716	-2.994	21.113	16.570	1.00	28.84
357	C	VAL	A	716	-2.687	19.683	17.037	1.00	36.83
358	O	VAL	A	716	-2.078	19.485	18.092	1.00	36.70
359	CB	VAL	A	716	-4.508	21.331	16.403	1.00	34.61

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
360	CG1	VAL	A	716	-5.239	20.839	17.647	1.00	29.84
361	CG2	VAL	A	716	-4.805	22.811	16.185	1.00	32.32
362	N	LYS	A	717	-2.972	18.709	16.179	1.00	38.71
363	CA	LYS	A	717	-2.737	17.313	16.505	1.00	32.14
364	C	LYS	A	717	-1.263	16.990	16.699	1.00	32.82
365	O	LYS	A	717	-0.920	16.262	17.631	1.00	34.86
366	CB	LYS	A	717	-3.370	16.410	15.450	1.00	32.30
367	CG	LYS	A	717	-4.890	16.352	15.569	1.00	38.88
368	CD	LYS	A	717	-5.538	15.584	14.436	0.00	36.05
369	CE	LYS	A	717	-7.009	15.353	14.736	0.00	36.14
370	NZ	LYS	A	717	-7.739	14.704	13.619	0.00	35.32
371	N	TRP	A	718	-0.383	17.589	15.893	1.00	31.69
372	CA	TRP	A	718	1.058	17.319	16.010	1.00	34.84
373	C	TRP	A	718	1.604	17.753	17.367	1.00	44.15
374	O	TRP	A	718	2.347	17.014	18.020	1.00	48.94
375	CB	TRP	A	718	1.850	17.995	14.883	1.00	25.87
376	CG	TRP	A	718	3.343	18.092	15.136	1.00	25.59
377	CD1	TRP	A	718	4.279	17.133	14.909	1.00	35.87
378	CD2	TRP	A	718	4.055	19.232	15.641	1.00	30.45
379	NE1	TRP	A	718	5.533	17.598	15.237	1.00	32.13
380	CE2	TRP	A	718	5.419	18.889	15.689	1.00	30.51
381	CE3	TRP	A	718	3.672	20.519	16.046	1.00	32.20
382	CZ2	TRP	A	718	6.403	19.782	16.119	1.00	32.90
383	CZ3	TRP	A	718	4.650	21.408	16.468	1.00	25.41
384	CH2	TRP	A	718	5.997	21.036	16.503	1.00	28.69
385	N	ALA	A	719	1.242	18.973	17.764	1.00	56.34
386	CA	ALA	A	719	1.654	19.580	19.037	1.00	52.43
387	C	ALA	A	719	1.176	18.846	20.305	1.00	47.73
388	O	ALA	A	719	1.968	18.662	21.246	1.00	46.60
389	CB	ALA	A	719	1.214	21.043	19.073	1.00	48.46
390	N	LYS	A	720	-0.107	18.461	20.337	1.00	42.77
391	CA	LYS	A	720	-0.697	17.744	21.478	1.00	45.06
392	C	LYS	A	720	-0.019	16.386	21.772	1.00	47.46
393	O	LYS	A	720	-0.227	15.789	22.835	1.00	50.10
394	CB	LYS	A	720	-2.218	17.567	21.294	1.00	39.13
395	CG	LYS	A	720	-3.057	18.632	21.979	1.00	45.90
396	CD	LYS	A	720	-4.533	18.253	22.075	1.00	55.06

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	397	CE	LYS	A	720	-5.236	19.088	23.161	1.00	63.65
	398	NZ	LYS	A	720	-6.668	18.719	23.402	1.00	62.72
	399	N	ALA	A	721	0.810	15.926	20.842	1.00	40.80
10	400	CA	ALA	A	721	1.524	14.671	20.995	1.00	41.77
	401	C	ALA	A	721	2.991	14.884	21.346	1.00	41.79
	402	O	ALA	A	721	3.762	13.931	21.370	1.00	43.57
15	403	CB	ALA	A	721	1.410	13.840	19.710	1.00	45.25
	404	N	LEU	A	722	3.382	16.131	21.585	1.00	40.71
	405	CA	LEU	A	722	4.764	16.438	21.927	1.00	34.69
20	406	C	LEU	A	722	5.115	16.085	23.369	1.00	33.82
	407	O	LEU	A	722	4.301	16.249	24.281	1.00	34.39
	408	CB	LEU	A	722	5.058	17.911	21.665	1.00	32.26
25	409	CG	LEU	A	722	5.357	18.244	20.218	1.00	33.93
	410	CD1	LEU	A	722	5.226	19.728	20.021	1.00	43.98
	411 1	CD2	LEU	A	722	6.753	17.784	19.880	1.00	30.81
30	412	N	PRO	A	723	6.338	15.589	23.592	1.00	37.66
	413	CA	PRO	A	723	6.820	15.209	24.917	1.00	35.69
	414	C	PRO	A	723	6.724	16.368	25.893	1.00	39.06
35	415	O	PRO	A	723	7.512	17.304	25.833	1.00	39.26
	416	CB	PRO	A	723	8.285	14.855	24.662	1.00	34.40
	417	CG	PRO	A	723	8.272	14.339	23.283	1.00	36.44
40	418	CD	PRO	A	723	7.354	15.282	22.562	1.00	41.22
	419	N	GLY	A	724	5.780	16.284	26.812	1.00	39.75
	420	CA	GLY	A	724	5.652	17.336	27.794	1.00	34.24
45	421	C	GLY	A	724	4.544	18.311	27.480	1.00	36.36
	422	O	GLY	A	724	3.911	18.837	28.398	1.00	37.90
	423	N	PHE	A	725	4.212	18.465	26.201	1.00	32.86
50	424	CA	PHE	A	725	3.192	19.422	25.845	1.00	36.30
	425	C	PHE	A	725	1.899	19.385	26.620	1.00	41.59
	426	O	PHE	A	725	1.385	20.441	27.002	1.00	44.02
55	427	CB	PHE	A	725	2.842	19.365	24.383	1.00	32.46
	428	CG	PHE	A	725	1.928	20.474	23.958	1.00	37.13
	429	CD1	PHE	A	725	2.453	21.687	23.542	1.00	37.70
55	430	CD2	PHE	A	725	0.544	20.302	23.948	1.00	39.17
	431	CE1	PHE	A	725	1.618	22.717	23.107	1.00	36.54
	432	CE2	PHE	A	725	-0.308	21.331	23.513	1.00	39.69
	433	CZ	PHE	A	725	0.233	22.540	23.089	1.00	42.41

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	434	N	ARG	A	726	1.335	18.189	26.791	1.00	49.80
	435	CA	ARG	A	726	0.050	18.042	27.489	1.00	49.46
	436	C	ARG	A	726	0.057	18.304	28.995	1.00	52.43
10	437	O	ARG	A	726	-0.978	18.139	29.644	1.00	52.56
	438	CB	ARG	A	726	-0.652	16.709	27.154	1.00	44.05
	439	CG	ARG	A	726	-1.692	16.821	26.023	1.00	44.55
	440	CD	ARG	A	726	-2.598	15.606	26.003	1.00	48.35
15	441	NE	ARG	A	726	-3.771	15.752	25.130	1.00	56.42
	442	CZ	ARG	A	726	-5.040	15.569	25.526	1.00	62.91
	443	NH1	ARG	A	726	-5.323	15.249	26.799	1.00	55.81
20	444	NH2	ARG	A	726	-6.028	15.649	24.632	1.00	55.35
	445	N	ASN	A	727	1.213	18.685	29.551	1.00	53.84
	446	CA	ASN	A	727	1.292	19.018	30.969	1.00	58.03
	447	C	ASN	A	727	1.026	20.528	31.138	1.00	61.72
25	448	O	ASN	A	727	0.723	20.993	32.248	1.00	65.35
	449	CB	ASN	A	727	2.636	18.589	31.604	1.00	63.66
	450	CG	ASN	A	727	3.777	19.597	31.388	1.00	67.51
30	451	OD1	ASN	A	727	4.837	19.234	30.881	1.00	68.14
	452	ND2	ASN	A	727	3.606	20.828	31.864	1.00	73.64
	453	N	LEU	A	728	1.190	21.288	30.047	1.00	59.72
	454	CA	LEU	A	728	0.957	22.739	30.035	1.00	50.93
35	455	C	LEU	A	728	-0.520	23.033	30.227	1.00	47.17
	456	O	LEU	A	728	-1.365	22.247	29.822	1.00	45.55
	457	CB	LEU	A	728	1.369	23.348	28.695	1.00	54.70
40	458	CG	LEU	A	728	2.822	23.408	28.228	1.00	52.07
	459	CD1	LEU	A	728	2.808	24.029	26.844	1.00	45.38
	460	CD2	LEU	A	728	3.700	24.223	29.181	1.00	47.21
	461	N	HIS	A	729	-0.841	24.201	30.763	1.00	45.54
45	462	CA	HIS	A	729	-2.231	24.530	30.986	1.00	44.10
	463	C	HIS	A	729	-2.972	24.559	29.655	1.00	40.23
	464	O	HIS	A	729	-2.421	24.976	28.658	1.00	44.09
50	465	CB	HIS	A	729	-2.328	25.851	31.716	1.00	54.55
	466	CG	HIS	A	729	-3.717	26.221	32.119	1.00	63.22
	467	ND1	HIS	A	729	-4.016	26.777	33.340	1.00	63.71
	468	CD2	HIS	A	729	-4.893	26.156	31.442	1.00	66.57
55	469	CE1	HIS	A	729	-5.308	27.046	33.401	1.00	68.21
	470	NE2	HIS	A	729	-5.861	26.678	32.256	1.00	68.48

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
471	N	VAL	A	730	-4.224	24.116	29.653	1.00	39.50
472	CA	VAL	A	730	-5.024	24.042	28.433	1.00	42.50
473	C	VAL	A	730	-5.016	25.262	27.563	1.00	45.07
474	O	VAL	A	730	-4.893	25.178	26.339	1.00	50.12
475	CB	VAL	A	730	-6.500	23.653	28.710	1.00	50.67
476	CG1	VAL	A	730	-7.044	24.387	29.936	1.00	48.50
477	CG2	VAL	A	730	-7.367	23.960	27.478	1.00	50.44
478	N	ASP	A	731	-5.249	26.399	28.185	1.00	51.13
479	CA	ASP	A	731	-5.269	27.646	27.453	1.00	51.89
480	C	ASP	A	731	-3.856	27.909	26.971	1.00	46.10
481	O	ASP	A	731	-3.663	28.213	25.810	1.00	51.50
482	CB	ASP	A	731	-5.820	28.755	28.338	1.00	51.89
483	CG	ASP	A	731	-7.194	28.415	28.872	1.00	59.37
484	OD1	ASP	A	731	-8.065	28.082	28.030	1.00	56.09
485	OD2	ASP	A	731	-7.373	28.414	30.122	1.00	61.65
486	N	ASP	A	732	-2.862	27.675	27.814	1.00	37.19
487	CA	ASP	A	732	-1.482	27.861	27.392	1.00	37.51
488	C	ASP	A	732	-1.177	26.934	26.232	1.00	39.98
489	O	ASP	A	732	-0.398	27.268	25.351	1.00	44.52
490	CB	ASP	A	732	-0.516	27.597	28.536	1.00	40.29
491	CG	ASP	A	732	-0.523	28.713	29.565	1.00	51.89
492	OD1	ASP	A	732	-1.171	29.755	29.313	1.00	56.09
493	OD2	ASP	A	732	0.116	28.562	30.631	1.00	59.50
494	N	GLN	A	733	-1.819	25.776	26.213	1.00	46.01
495	CA	GLN	A	733	-1.621	24.832	25.131	1.00	48.12
496	C	GLN	A	733	-2.183	25.485	23.884	1.00	48.61
497	O	GLN	A	733	-1.531	25.558	22.854	1.00	51.31
498	CB	GLN	A	733	-2.421	23.563	25.364	1.00	52.94
499	CG	GLN	A	733	-1.791	22.511	26.234	1.00	52.25
500	CD	GLN	A	733	-2.659	21.287	26.227	1.00	53.92
501	OE1	GLN	A	733	-3.252	20.925	27.238	1.00	59.82
502	NE2	GLN	A	733	-2.836	20.701	25.051	1.00	55.07
503	N	MET	A	734	-3.416	25.952	23.993	1.00	48.02
504	CA	MET	A	734	-4.107	26.588	22.887	1.00	50.74
505	C	MET	A	734	-3.448	27.904	22.453	1.00	50.43
506	O	MET	A	734	-3.495	28.269	21.286	1.00	53.47
507	CB	MET	A	734	-5.545	26.832	23.297	1.00	56.63

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
508	CG	MET	A	734	-6.530	26.884	22.158	1.00	71.95
509	SD	MET	A	734	-8.226	26.806	22.797	1.00	94.18
510	CE	MET	A	734	-7.929	26.442	24.662	1.00	83.04
511 1	N	ALA	A	735	-2.779	28.577	23.384	1.00	49.75
512	CA	ALA	A	735	-2.115	29.844	23.109	1.00	43.40
513	C	ALA	A	735	-0.820	29.686	22.305	1.00	43.42
514	O	ALA	A	735	-0.749	30.185	21.185	1.00	51.41
515	CB	ALA	A	735	-1.845	30.602	24.406	1.00	36.08
516	N	VAL	A	736	0.198	29.002	22.832	1.00	38.22
517	CA	VAL	A	736	1.441	28.866	22.066	1.00	36.45
518	C	VAL	A	736	1.210	28.345	20.651	1.00	36.01
519	O	VAL	A	736	1.982	28.655	19.747	1.00	41.42
520	CB	VAL	A	736	2.502	28.000	22.764	1.00	35.87
521	CG1	VAL	A	736	3.048	28.714	23.978	1.00	44.32
522	CG2	VAL	A	736	1.924	26.673	23.156	1.00	36.64
523	N	ILE	A	737	0.132	27.585	20.465	1.00	30.08
524	CA	ILE	A	737	-0.220	27.048	19.150	1.00	31.25
525	C	ILE	A	737	-0.623	28.195	18.241	1.00	32.22
526	O	ILE	A	737	0.022	28.449	17.222	1.00	40.26
527	CB	ILE	A	737	-1.361	25.992	19.250	1.00	32.49
528	CG1	ILE	A	737	-0.781	24.654	19.749	1.00	36.28
529	CG2	ILE	A	737	-2.061	25.803	17.907	1.00	22.38
530	CD1	ILE	A	737	-1.792	23.707	20.422	1.00	39.52
531	N	GLN	A	738	-1.657	28.926	18.636	1.00	34.76
532	CA	GLN	A	738	-2.127	30.064	17.857	1.00	36.96
533	C	GLN	A	738	-0.999	31.078	17.575	1.00	38.78
534	O	GLN	A	738	-0.780	31.434	16.422	1.00	47.01
535	CB	GLN	A	738	-3.310	30.715	18.570	1.00	35.31
536	CG	GLN	A	738	-4.548	29.817	18.615	1.00	36.30
537	CD	GLN	A	738	-5.569	30.254	19.666	1.00	46.43
538	OE1	GLN	A	738	-5.196	30.752	20.728	1.00	51.09
539	NE2	GLN	A	738	-6.860	30.059	19.379	1.00	45.97
540	N	TYR	A	739	-0.206	31.428	18.586	1.00	32.35
541	CA	TYR	A	739	0.867	32.387	18.402	1.00	30.36
542	C	TYR	A	739	1.975	31.867	17.526	1.00	34.27
543	O	TYR	A	739	2.502	32.609	16.712	1.00	35.19
544	CB	TYR	A	739	1.496	32.821	19.735	1.00	36.60

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	545	CG	TYR	A	739	0.565	33.487	20.754	1.00	41.72
	546	CD1	TYR	A	739	-0.515	34.267	20.358	1.00	43.18
	547	CD2	TYR	A	739	0.736	33.272	22.126	1.00	44.87
10	548	CE1	TYR	A	739	-1.416	34.803	21.303	1.00	43.31
	549	CE2	TYR	A	739	-0.163	33.808	23.073	1.00	39.98
	550	CZ	TYR	A	739	-1.239	34.561	22.649	1.00	38.00
15	551	OH	TYR	A	739	-2.178	35.014	23.556	1.00	54.08
	552	N	SER	A	740	2.351	30.606	17.674	1.00	36.52
	553	CA	SER	A	740	3.459	30.114	16.875	1.00	38.17
20	554	C	SER	A	740	3.129	29.453	15.535	1.00	38.14
	555	O	SER	A	740	4.024	29.259	14.706	1.00	41.67
	556	CB	SER	A	740	4.390	29.231	17.727	1.00	42.37
25	557	OG	SER	A	740	3.756	28.053	18.200	1.00	39.05
	558	N	TRP	A	741	1.851	29.268	15.236	1.00	32.00
	559	CA	TRP	A	741	1.482	28.588	14.004	1.00	32.79
30	560	C	TRP	A	741	2.099	29.060	12.681	1.00	34.24
	561	O	TRP	A	741	2.578	28.250	11.891	1.00	34.43
	562	CB	TRP	A	741	-0.034	28.446	13.918	1.00	44.21
35	563	CG	TRP	A	741	-0.733	29.487	13.136	1.00	58.12
	564	CD1	TRP	A	741	-0.889	30.806	13.458	1.00	64.16
	565	CD2	TRP	A	741	-1.365	29.303	11.870	1.00	63.13
40	566	NE1	TRP	A	741	-1.574	31.462	12.462	1.00	67.31
	567	CE2	TRP	A	741	-1.882	30.562	11.473	1.00	67.95
	568	CE3	TRP	A	741	-1.558	28.194	11.031	1.00	57.71
45	569	CZ2	TRP	A	741	-2.561	30.747	10.260	1.00	70.02
	570	CZ3	TRP	A	741	-2.232	28.373	9.831	1.00	59.16
	571	CH2	TRP	A	741	-2.731	29.642	9.458	1.00	65.30
50	572	N	MET	A	742	2.184	30.370	12.489	1.00	41.58
	573	CA	MET	A	742	2.749	30.945	11.265	1.00	39.13
	574	C	MET	A	742	4.193	30.537	11.090	1.00	30.85
55	575	O	MET	A	742	4.602	30.115	10.017	1.00	34.78
	576	CB	MET	A	742	2.689	32.476	11.309	1.00	42.39
	577	CG	MET	A	742	3.147	33.177	10.032	1.00	43.70
55	578	SD	MET	A	742	1.988	32.993	8.658	1.00	45.17
	579	CE	MET	A	742	0.678	34.132	9.133	1.00	22.14
	580	N	GLY	A	743	4.954	30.648	12.165	1.00	24.94
	581	CA	GLY	A	743	6.367	30.312	12.117	1.00	27.24

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
582	C	GLY	A	743	6.630	28.836	11.886	1.00	27.21
583	O	GLY	A	743	7.660	28.461	11.322	1.00	27.69
584	N	LEU	A	744	5.734	27.983	12.372	1.00	25.91
585	CA	LEU	A	744	5.895	26.550	12.172	1.00	26.90
586	C	LEU	A	744	5.632	26.287	10.708	1.00	27.04
587	O	LEU	A	744	6.375	25.574	10.048	1.00	31.01
588	CB	LEU	A	744	4.899	25.755	13.018	1.00	25.72
589	CG	LEU	A	744	5.234	25.626	14.514	1.00	29.11
590	CD1	LEU	A	744	4.063	25.022	15.275	1.00	23.25
591	CD2	LEU	A	744	6.484	24.771	14.689	1.00	24.15
592	N	MET	A	745	4.566	26.886	10.200	1.00	25.67
593	CA	MET	A	745	4.188	26.725	8.803	1.00	23.96
594	C	MET	A	745	5.254	27.179	7.822	1.00	29.61
595	O	MET	A	745	5.550	26.480	6.857	1.00	34.60
596	CB	MET	A	745	2.895	27.454	8.534	1.00	20.46
597	CG	MET	A	745	1.730	26.888	9.310	1.00	19.98
598	SD	MET	A	745	0.297	27.272	8.341	1.00	43.15
599	CE	MET	A	745	0.642	29.041	8.042	1.00	44.27
600	N	VAL	A	746	5.830	28.341	8.095	1.00	27.98
601	CA	VAL	A	746	6.876	28.924	7.288	1.00	24.84
602	C	VAL	A	746	8.107	28.051	7.345	1.00	28.42
603	O	VAL	A	746	8.749	27.786	6.333	1.00	37.05
604	CB	VAL	A	746	7.248	30.304	7.835	1.00	31.98
605	CG1	VAL	A	746	8.423	30.888	7.073	1.00	29.03
606	CG2	VAL	A	746	6.066	31.196	7.737	1.00	32.19
607	N	PHE	A	747	8.439	27.607	8.541	1.00	31.29
608	CA	PHE	A	747	9.605	26.765	8.736	1.00	32.19
609	C	PHE	A	747	9.468	25.401	8.030	1.00	35.99
610	O	PHE	A	747	10.398	24.916	7.384	1.00	34.95
611	CB	PHE	A	747	9.820	26.536	10.224	1.00	27.90
612	CG	PHE	A	747	11.209	26.082	10.573	1.00	26.00
613	CD1	PHE	A	747	12.293	26.915	10.343	1.00	24.54
614	CD2	PHE	A	747	11.428	24.846	11.166	1.00	27.23
615	CE1	PHE	A	747	13.571	26.532	10.699	1.00	25.88
616	CE2	PHE	A	747	12.711	24.451	11.528	1.00	25.61
617	CZ	PHE	A	747	13.785	25.297	11.293	1.00	28.75
618	N	ALA	A	748	8.309	24.774	8.171	1.00	35.11

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	619	CA	ALA	A	748	8.096	23.483	7.561	1.00	34.00
	620	C	ALA	A	748	8.114	23.683	6.054	1.00	37.26
	621	O	ALA	A	748	8.831	22.973	5.344	1.00	35.87
10	622	CB	ALA	A	748	6.773	22.896	8.022	1.00	29.48
	623	N	MET	A	749	7.385	24.707	5.591	1.00	41.15
	624	CA	MET	A	749	7.277	25.044	4.167	1.00	33.31
15	625	C	MET	A	749	8.647	25.225	3.563	1.00	35.12
	626	O	MET	A	749	8.934	24.711	2.491	1.00	37.94
	627	CB	MET	A	749	6.444	26.303	3.982	1.00	35.95
20	628	CG	MET	A	749	6.179	26.682	2.542	1.00	45.47
	629	SD	MET	A	749	7.444	27.726	1.821	1.00	50.89
	630	CE	MET	A	749	7.553	28.954	3.104	1.00	55.72
25	631	N	GLY	A	750	9.507	25.929	4.278	1.00	36.97
	632	CA	GLY	A	750	10.863	26.138	3.810	1.00	42.04
	633	C	GLY	A	750	11.628	24.828	3.715	1.00	43.22
30	634	O	GLY	A	750	12.530	24.678	2.889	1.00	43.48
	635	N	TRP	A	751	11.304	23.876	4.581	1.00	45.43
	636	CA	TRP	A	751	11.976	22.588	4.528	1.00	42.53
35	637	C	TRP	A	751	11.519	21.806	3.294	1.00	43.17
	638	O	TRP	A	751	12.336	21.207	2.596	1.00	40.24
	639	CB	TRP	A	751	11.717	21.776	5.787	1.00	39.21
40	640	CG	TRP	A	751	12.359	20.401	5.737	1.00	41.85
	641	CD1	TRP	A	751	11.736	19.213	5.461	1.00	39.44
	642	CD2	TRP	A	751	13.743	20.085	5.968	1.00	37.37
45	643	NE1	TRP	A	751	12.645	18.186	5.516	1.00	42.23
	644	CE2	TRP	A	751	13.878	18.692	5.821	1.00	41.26
	645	CE3	TRP	A	751	14.877	20.841	6.275	1.00	41.35
50	646	CZ2	TRP	A	751	15.110	18.046	5.978	1.00	48.39
	647	CZ3	TRP	A	751	16.104	20.195	6.431	1.00	39.62
	648	CH2	TRP	A	751	16.208	18.817	6.280	1.00	43.38
55	649	N	ARG	A	752	10.214	21.792	3.037	1.00	42.27
	650	CA	ARG	A	752	9.683	21.100	1.862	1.00	41.53
	651	C	ARG	A	752	10.257	21.740	0.602	1.00	44.18
55	652	O	ARG	A	752	10.522	21.048	-0.380	1.00	43.20
	653	CB	ARG	A	752	8.163	21.186	1.800	1.00	42.14
	654	CG	ARG	A	752	7.441	20.465	2.920	1.00	49.76
	655	CD	ARG	A	752	5.938	20.434	2.649	1.00	48.23

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5 656	NE	ARG	A	752	5.382	21.773	2.483	1.00	45.23
657	CZ	ARG	A	752	5.013	22.572	3.490	1.00	52.17
658	NH1	ARG	A	752	5.131	22.175	4.764	1.00	33.80
659	NH2	ARG	A	752	4.536	23.785	3.223	1.00	49.84
10 660	N	SER	A	753	10.441	23.058	0.624	1.00	38.26
661	CA	SER	A	753	10.998	23.733	-0.523	1.00	35.26
662	C	SER	A	753	12.453	23.400	-0.707	1.00	35.66
15 663	O	SER	A	753	12.973	23.538	-1.807	1.00	43.18
664	CB	SER	A	753	10.798	25.233	-0.444	1.00	33.49
665	OG	SER	A	753	9.414	25.514	-0.453	1.00	36.06
20 666	N	PHE	A	754	13.113	22.938	0.343	1.00	33.77
667	CA	PHE	A	754	14.523	22.575	0.224	1.00	41.59
668	C	PHE	A	754	14.709	21.153	-0.316	1.00	49.14
669	O	PHE	A	754	15.524	20.919	-1.211	1.00	48.97
25 670	CB	PHE	A	754	15.242	22.702	1.564	1.00	39.18
671	CG	PHE	A	754	16.668	22.204	1.540	1.00	40.02
672	CD1	PHE	A	754	17.596	22.746	0.645	1.00	48.31
30 673	CD2	PHE	A	754	17.086	21.202	2.423	1.00	36.75
674	CE1	PHE	A	754	18.923	22.311	0.635	1.00	47.66
675	CE2	PHE	A	754	18.411	20.757	2.432	1.00	41.02
676	CZ	PHE	A	754	19.333	21.313	1.532	1.00	50.13
35 677	N	THR	A	755	13.948	20.208	0.225	1.00	53.24
678	CA	THR	A	755	14.053	18.818	-0.197	1.00	53.33
679	C	THR	A	755	13.287	18.474	-1.478	1.00	54.87
40 680	O	THR	A	755	13.554	17.431	-2.068	1.00	57.41
681	CB	THR	A	755	13.596	17.830	0.934	1.00	45.98
682	OG1	THR	A	755	12.221	18.055	1.245	1.00	49.35
683	CG2	THR	A	755	14.405	18.033	2.190	1.00	40.03
45 684	N	ASN	A	756	12.360	19.336	-1.911	1.00	52.97
685	CA	ASN	A	756	11.539	19.044	-3.097	1.00	56.15
686	C	ASN	A	756	11.821	19.826	-4.394	1.00	55.33
50 687	O	ASN	A	756	11.705	19.257	-5.481	1.00	54.81
688	CB	ASN	A	756	10.019	19.124	-2.769	1.00	60.43
689	CG	ASN	A	756	9.504	17.959	-1.869	1.00	57.82
690	OD1	ASN	A	756	10.123	16.909	-1.763	1.00	55.71
55 691	ND2	ASN	A	756	8.354	18.169	-1.234	1.00	56.46
692	N	VAL	A	757	12.155	21.115	-4.293	1.00	54.53

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	693	CA	VAL	A	757	12.427	21.962	-5.470	1.00	50.64
	694	C	VAL	A	757	13.732	22.776	-5.370	1.00	47.30
	695	O	VAL	A	757	13.903	23.786	-6.053	1.00	48.03
10	696	CB	VAL	A	757	11.239	22.943	-5.756	1.00	50.94
	697	CG1	VAL	A	757	9.927	22.177	-5.892	1.00	53.22
	698	CG2	VAL	A	757	11.125	23.998	-4.660	1.00	54.28
15	699	N	ASN	A	758	14.676	22.274	-4.582	1.00	53.28
	700	CA	ASN	A	758	15.977	22.917	-4.340	1.00	61.04
	701	C	ASN	A	758	15.937	24.448	-4.140	1.00	63.53
20	702	O	ASN	A	758	16.674	25.191	-4.802	1.00	65.98
	703	CB	ASN	A	758	17.026	22.499	-5.388	1.00	63.98
	704	CG	ASN	A	758	18.440	22.442	-4.813	1.00	62.08
25	705	OD1	ASN	A	758	18.681	22.852	-3.679	0.00	62.62
	706	ND2	ASN	A	758	19.369	21.908	-5.590	0.00	62.48
	707	N	SER	A	759	14.999	24.879	-3.281	1.00	63.72
30	708	CA	SER	A	759	14.763	26.267	-2.849	1.00	61.29
	709	C	SER	A	759	14.379	27.351	-3.849	1.00	66.13
	710	O	SER	A	759	14.067	28.472	-3.443	1.00	71.37
35	711	CB	SER	A	759	15.939	26.770	-1.995	1.00	60.64
	712	OG	SER	A	759	16.080	26.018	-0.799	1.00	55.92
	713	N	ARG	A	760	14.388	27.045	-5.140	1.00	64.35
40	714	CA	ARG	A	760	14.041	28.064	-6.109	1.00	59.78
	715	C	ARG	A	760	12.551	28.416	-6.070	1.00	55.67
	716	O	ARG	A	760	12.186	29.563	-6.345	1.00	60.84
45	717	CB	ARG	A	760	14.492	27.658	-7.507	1.00	69.19
	718	CG	ARG	A	760	14.046	26.283	-7.883	1.00	73.58
	719	CD	ARG	A	760	13.925	26.094	-9.381	1.00	78.27
50	720	NE	ARG	A	760	13.214	24.847	-9.635	1.00	80.85
	721	CZ	ARG	A	760	13.642	23.646	-9.246	1.00	80.46
	722	NH1	ARG	A	760	14.801	23.528	-8.597	1.00	79.19
55	723	NH2	ARG	A	760	12.853	22.584	-9.388	1.00	76.84
	724	N	MET	A	761	11.701	27.453	-5.707	1.00	46.97
	725	CA	MET	A	761	10.256	27.695	-5.622	1.00	41.01
55	726	C	MET	A	761	9.744	27.418	-4.222	1.00	37.53
	727	O	MET	A	761	10.451	26.824	-3.412	1.00	38.47
	728	CB	MET	A	761	9.496	26.827	-6.612	1.00	38.49
	729	CG	MET	A	761	9.926	27.040	-8.034	1.00	42.52

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
730	SD	MET	A	761	8.981	25.994	-9.104	1.00	50.12
731	CE	MET	A	761	10.000	24.558	-9.111	1.00	43.61
732	N	LEU	A	762	8.526	27.860	-3.930	1.00	35.00
733	CA	LEU	A	762	7.949	27.638	-2.614	1.00	36.81
734	C	LEU	A	762	6.902	26.548	-2.664	1.00	41.13
735	O	LEU	A	762	5.821	26.739	-3.243	1.00	36.62
736	CB	LEU	A	762	7.344	28.912	-2.048	1.00	39.16
737	CG	LEU	A	762	8.366	30.021	-1.827	1.00	43.49
738	CD1	LEU	A	762	7.670	31.178	-1.169	1.00	45.89
739	CD2	LEU	A	762	9.498	29.530	-0.952	1.00	44.69
740	N	TYR	A	763	7.245	25.419	-2.033	1.00	44.41
741	CA	TYR	A	763	6.422	24.209	-1.963	1.00	39.75
742	C	TYR	A	763	5.412	24.241	-0.839	1.00	36.53
743	O	TYR	A	763	5.504	23.487	0.129	1.00	36.31
744	CB	TYR	A	763	7.323	22.968	-1.831	1.00	47.60
745	CG	TYR	A	763	6.713	21.644	-2.309	1.00	61.61
746	CD1	TYR	A	763	5.701	21.002	-1.579	1.00	67.78
747	CD2	TYR	A	763	7.174	21.015	-3.476	1.00	62.67
748	CE1	TYR	A	763	5.164	19.770	-1.998	1.00	63.34
749	CE2	TYR	A	763	6.639	19.778	-3.897	1.00	59.80
750	CZ	TYR	A	763	5.634	19.173	-3.149	1.00	62.05
751	OH	TYR	A	763	5.066	17.995	-3.558	1.00	63.40
752	N	PHE	A	764	4.445	25.130	-0.958	1.00	37.20
753	CA	PHE	A	764	3.409	25.221	0.042	1.00	38.87
754	C	PHE	A	764	2.681	23.864	0.164	1.00	47.03
755	O	PHE	A	764	2.506	23.333	1.263	1.00	48.96
756	CB	PHE	A	764	2.441	26.350	-0.321	1.00	34.03
757	CG	PHE	A	764	3.048	27.695	-0.225	1.00	29.36
758	CD1	PHE	A	764	3.571	28.142	0.976	1.00	32.46
759	CD2	PHE	A	764	3.129	28.510	-1.328	1.00	37.55
760	CE1	PHE	A	764	4.169	29.384	1.076	1.00	35.80
761	CE2	PHE	A	764	3.727	29.759	-1.236	1.00	39.68
762	CZ	PHE	A	764	4.247	30.196	-0.033	1.00	29.54
763	N	ALA	A	765	2.314	23.286	-0.978	1.00	56.26
764	CA	ALA	A	765	1.608	21.999	-1.049	1.00	51.43
765	C	ALA	A	765	1.969	21.343	-2.386	1.00	51.42
766	O	ALA	A	765	2.449	22.022	-3.289	1.00	51.71

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	767	CB	ALA	A	765	0.105	22.232	-0.959	1.00	47.80
	768	N	PRO	A	766	1.766	20.021	-2.533	1.00	52.86
	769	CA	PRO	A	766	2.120	19.407	-3.813	1.00	50.96
10	770	C	PRO	A	766	1.359	20.040	-4.970	1.00	48.25
	771	O	PRO	A	766	1.893	20.144	-6.082	1.00	44.31
	772	CB	PRO	A	766	1.721	17.949	-3.604	1.00	57.00
15	773	CG	PRO	A	766	1.899	17.761	-2.133	1.00	58.08
	774	CD	PRO	A	766	1.237	19.002	-1.617	1.00	57.23
	775	N	ASP	A	767	0.128	20.479	-4.707	1.00	41.59
20	776	CA	ASP	A	767	-0.681	21.119	-5.743	1.00	47.13
	777	C	ASP	A	767	-0.774	22.666	-5.645	1.00	51.59
	778	O	ASP	A	767	-1.618	23.311	-6.292	1.00	55.70
25	779	CB	ASP	A	767	-2.073	20.485	-5.785	1.00	48.65
	780	CG	ASP	A	767	-2.833	20.667	-4.505	1.00	51.77
	781	OD1	ASP	A	767	-2.205	20.619	-3.431	1.00	54.76
30	782	OD2	ASP	A	767	-4.071	20.839	-4.573	1.00	59.43
	783	N	LEU	A	768	0.148	23.255	-4.893	1.00	48.07
	784	CA	LEU	A	768	0.196	24.697	-4.719	1.00	47.04
35	785	C	LEU	A	768	1.658	25.080	-4.564	1.00	49.99
	786	O	LEU	A	768	2.141	25.212	-3.436	1.00	53.64
	787	CB	LEU	A	768	-0.574	25.108	-3.450	1.00	51.86
40	788	CG	LEU	A	768	-0.631	26.580	-3.002	1.00	50.53
	789	CD1	LEU	A	768	-1.328	27.390	-4.062	1.00	47.97
	790	CD2	LEU	A	768	-1.376	26.701	-1.702	1.00	46.42
45	791	N	VAL	A	769	2.387	25.176	-5.676	1.00	48.70
	792	CA	VAL	A	769	3.796	25.575	-5.620	1.00	48.86
	793	C	VAL	A	769	3.954	26.933	-6.287	1.00	47.94
50	794	O	VAL	A	769	3.352	27.190	-7.335	1.00	49.55
	795	CB	VAL	A	769	4.728	24.572	-6.321	1.00	50.85
	796	CG1	VAL	A	769	6.181	25.049	-6.216	1.00	53.54
55	797	CG2	VAL	A	769	4.581	23.208	-5.687	1.00	53.42
	798	N	PHE	A	770	4.734	27.808	-5.668	1.00	43.61
	799	CA	PHE	A	770	4.935	29.124	-6.230	1.00	40.71
	800	C	PHE	A	770	6.179	29.276	-7.044	1.00	39.27
	801	O	PHE	A	770	7.291	29.151	-6.531	1.00	38.13
	802	CB	PHE	A	770	4.939	30.197	-5.147	1.00	41.24
	803	CG	PHE	A	770	3.582	30.650	-4.753	1.00	39.60

TABLE 9 (continued)

TABLE 9 (continued)										
THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	804	CD1	PHE	A	770	2.489	29.803	-4.896	1.00	40.94
	805	CD2	PHE	A	770	3.391	31.916	-4.220	1.00	35.47
	806	CE1	PHE	A	770	1.216	30.208	-4.515	1.00	39.80
	807	CE2	PHE	A	770	2.123	32.332	-3.834	1.00	37.83
10	808	CZ	PHE	A	770	1.027	31.476	-3.980	1.00	36.48
	809	N	ASN	A	771	5.988	29.397	-8.345	1.00	38.22
	810	CA	ASN	A	771	7.113	29.673	-9.219	1.00	39.10
15	811	C	ASN	A	771	7.181	31.196	-9.066	1.00	43.17
	812	O	ASN	A	771	6.341	31.785	-8.345	1.00	39.83
	813	CB	ASN	A	771	6.834	29.268	-10.685	1.00	33.28
20	814	CG	ASN	A	771	5.384	29.492	-11.110	1.00	35.37
	815	OD1	ASN	A	771	4.656	30.309	-10.546	1.00	45.29
	816	ND2	ASN	A	771	4.956	28.737	-12.094	1.00	41.79
	817	N	GLU	A	772	8.166	31.836	-9.694	1.00	43.13
25	818	CA	GLU	A	772	8.264	33.285	-9.605	1.00	42.44
	819	C	GLU	A	772	7.015	33.997	-10.136	1.00	45.81
	820	O	GLU	A	772	6.615	35.016	-9.579	1.00	53.45
30	821	CB	GLU	A	772	9.541	33.815	-10.274	1.00	52.58
	822	CG	GLU	A	772	10.814	33.657	-9.401	1.00	58.43
	823	CD	GLU	A	772	11.791	34.850	-9.483	1.00	56.79
	824	OE1	GLU	A	772	11.719	35.655	-10.434	1.00	55.14
35	825	OE2	GLU	A	772	12.654	34.974	-8.583	1.00	61.19
	826	N	TYR	A	773	6.354	33.454	-11.157	1.00	39.45
	827	CA	TYR	A	773	5.147	34.117	-11.659	1.00	38.06
40	828	C	TYR	A	773	4.088	34.215	-10.565	1.00	38.71
	829	O	TYR	A	773	3.493	35.271	-10.391	1.00	41.42
	830	CB	TYR	A	773	4.563	33.425	-12.907	1.00	37.63
45	831	CG	TYR	A	773	3.266	34.033	-13.417	1.00	38.44
	832	CD1	TYR	A	773	3.248	35.277	-14.059	1.00	36.94
	833	CD2	TYR	A	773	2.043	33.397	-13.197	1.00	40.91
	834	CE1	TYR	A	773	2.038	35.883	-14.459	1.00	34.34
50	835	CE2	TYR	A	773	0.833	33.990	-13.595	1.00	46.98
	836	CZ	TYR	A	773	0.835	35.235	-14.223	1.00	42.85
	837	OH	TYR	A	773	-0.361	35.824	-14.599	1.00	42.16
55	838	N	ARG	A	774	3.864	33.137	-9.817	1.00	43.58
	839	CA	ARG	A	774	2.863	33.146	-8.751	1.00	41.94
	840	C	ARG	A	774	3.216	34.035	-7.578	1.00	41.03

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	841	O	ARG	A	774	2.330	34.701	-7.032	1.00	43.75
	842	CB	ARG	A	774	2.580	31.748	-8.252	1.00	46.64
	843	CG	ARG	A	774	1.421	31.121	-8.923	1.00	45.32
10	844	CD	ARG	A	774	1.735	29.667	-9.102	1.00	47.16
	845	NE	ARG	A	774	0.588	28.968	-9.642	1.00	43.73
	846	CZ	ARG	A	774	0.344	27.682	-9.445	1.00	41.94
15	847	NH1	ARG	A	774	1.183	26.954	-8.717	1.00	42.65
	848	NH2	ARG	A	774	-0.753	27.136	-9.952	1.00	39.92
	849	N	MET	A	775	4.486	34.023	-7.168	1.00	34.68
20	850	CA	MET	A	775	4.955	34.877	-6.069	1.00	38.36
	851	C	MET	A	775	4.496	36.328	-6.332	1.00	41.88
	852	O	MET	A	775	4.119	37.065	-5.416	1.00	41.28
25	853	CB	MET	A	775	6.485	34.839	-5.975	1.00	33.18
	854	CG	MET	A	775	7.046	33.622	-5.276	1.00	24.32
	855	SD	MET	A	775	8.813	33.416	-5.539	1.00	40.19
30	856	CE	MET	A	775	9.443	34.965	-4.970	1.00	48.34
	857	N	HIS	A	776	4.484	36.695	-7.608	1.00	46.87
	858	CA	HIS	A	776	4.065	38.006	-8.065	1.00	41.06
35	859	C	HIS	A	776	2.568	38.136	-8.311	1.00	43.18
	860	O	HIS	A	776	1.969	39.153	-7.991	1.00	48.98
	861	CB	HIS	A	776	4.804	38.351	-9.348	1.00	45.79
40	862	CG	HIS	A	776	4.486	39.712	-9.873	1.00	44.99
	863	ND1	HIS	A	776	3.327	39.992	-10.560	1.00	46.34
	864	CD2	HIS	A	776	5.167	40.879	-9.788	1.00	44.43
45	865	CE1	HIS	A	776	3.300	41.270	-10.877	1.00	44.55
	866	NE2	HIS	A	776	4.406	41.833	-10.419	1.00	49.86
	867	N	LYS	A	777	1.964	37.143	-8.938	1.00	46.29
50	868	CA	LYS	A	777	0.542	37.214	-9.220	1.00	48.46
	869	C	LYS	A	777	-0.276	37.241	-7.920	1.00	49.12
	870	O	LYS	A	777	-1.356	37.835	-7.869	1.00	53.96
55	871	CB	LYS	A	777	0.128	36.042	-10.126	1.00	50.10
	872	CG	LYS	A	777	-1.193	36.233	-10.872	1.00	58.08
	873	CD	LYS	A	777	-1.161	37.460	-11.791	1.00	65.16
55	874	CE	LYS	A	777	-2.090	38.590	-11.301	1.00	75.26
	875	NZ	LYS	A	777	-3.524	38.363	-11.635	1.00	77.33
	876	N	SER	A	778	0.249	36.616	-6.870	1.00	50.25
	877	CA	SER	A	778	-0.432	36.551	-5.571	1.00	48.63

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
878	C	SER	A	778	-0.193	37.808	-4.756	1.00	53.35
879	O	SER	A	778	-0.827	38.019	-3.727	1.00	57.00
880	CB	SER	A	778	0.116	35.397	-4.761	1.00	42.58
881	OG	SER	A	778	1.446	35.715	-4.386	1.00	43.83
882	N	ARG	A	779	0.842	38.546	-5.141	1.00	58.37
883	CA	ARG	A	779	1.242	39.798	-4.491	1.00	56.74
884	C	ARG	A	779	1.901	39.668	-3.113	1.00	54.76
885	O	ARG	A	779	1.801	40.580	-2.276	1.00	51.96
886	CB	ARG	A	779	0.081	40.799	-4.461	1.00	57.70
887	CG	ARG	A	779	-0.472	41.124	-5.841	1.00	56.33
888	CD	ARG	A	779	-1.603	42.120	-5.735	1.00	58.79
889	NE	ARG	A	779	-2.471	42.088	-6.907	1.00	62.79
890	CZ	ARG	A	779	-3.095	43.150	-7.397	1.00	61.40
891	NH1	ARG	A	779	-2.935	44.337	-6.824	1.00	62.02
892	NH2	ARG	A	779	-3.912	43.007	-8.426	1.00	65.13
893	N	MET	A	780	2.600	38.551	-2.897	1.00	46.79
894	CA	MET	A	780	3.323	38.334	-1.650	1.00	42.92
895	C	MET	A	780	4.773	38.214	-2.049	1.00	41.04
896	O	MET	A	780	5.595	37.686	-1.311	1.00	43.38
897	CB	MET	A	780	2.953	37.015	-1.005	1.00	45.45
898	CG	MET	A	780	1.530	36.831	-0.596	1.00	54.10
899	SD	MET	A	780	1.554	35.622	0.748	1.00	62.75
900	CE	MET	A	780	2.616	34.289	0.007	1.00	62.66
901	N	TYR	A	781	5.092	38.712	-3.229	1.00	39.62
902	CA	TYR	A	781	6.429	38.610	-3.744	1.00	33.06
903	C	TYR	A	781	7.532	38.923	-2.753	1.00	33.20
904	O	TYR	A	781	8.499	38.166	-2.682	1.00	40.06
905	CB	TYR	A	781	6.581	39.428	-5.019	1.00	33.87
906	CG	TYR	A	781	7.782	38.995	-5.819	1.00	46.69
907	CD1	TYR	A	781	9.063	39.330	-5.400	1.00	53.38
908	CD2	TYR	A	781	7.651	38.203	-6.952	1.00	48.14
909	CE1	TYR	A	781	10.184	38.887	-6.071	1.00	50.46
910	CE2	TYR	A	781	8.778	37.756	-7.644	1.00	46.86
911	CZ	TYR	A	781	10.051	38.105	-7.190	1.00	51.34
912	OH	TYR	A	781	11.207	37.679	-7.825	1.00	55.86
913	N	SER	A	782	7.419	40.009	-1.986	1.00	39.72
914	CA	SER	A	782	8.492	40.346	-1.009	1.00	46.33

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	915	C	SER	A	782	8.597	39.361	0.159	1.00	38.58
	916	O	SER	A	782	9.697	39.007	0.604	1.00	34.19
	917	CB	SER	A	782	8.364	41.780	-0.472	1.00	44.39
10	918	OG	SER	A	782	7.042	42.049	-0.044	1.00	52.83
	919	N	GLN	A	783	7.453	38.904	0.650	1.00	36.42
	920	CA	GLN	A	783	7.486	37.948	1.736	1.00	43.09
15	921	C	GLN	A	783	8.040	36.661	1.160	1.00	41.26
	922	O	GLN	A	783	8.980	36.075	1.709	1.00	47.55
	923	CB	GLN	A	783	6.102	37.717	2.321	1.00	42.73
20	924	CG	GLN	A	783	5.538	38.915	3.059	1.00	48.39
	925	CD	GLN	A	783	5.113	40.045	2.137	1.00	50.96
	926	OE1	GLN	A	783	4.504	39.831	1.083	1.00	53.94
25	927	NE2	GLN	A	783	5.430	41.260	2.538	1.00	52.89
	928	N	CYS	A	784	7.532	36.300	-0.015	1.00	36.76
	929	CA	CYS	A	784	7.945	35.084	-0.710	1.00	35.38
30	930	C	CYS	A	784	9.456	35.006	-0.859	1.00	33.10
	931	O	CYS	A	784	10.073	33.978	-0.568	1.00	39.32
	932	CB	CYS	A	784	7.244	34.989	-2.066	1.00	31.26
35	933	SG	CYS	A	784	5.513	34.425	-1.949	1.00	42.23
	934	N	VAL	A	785	10.060	36.132	-1.199	1.00	33.87
	935	CA	VAL	A	785	11.491	36.173	-1.363	1.00	31.80
40	936	C	VAL	A	785	12.149	35.937	-0.019	1.00	33.12
	937	O	VAL	A	785	13.164	35.267	0.051	1.00	35.91
	938	CB	VAL	A	785	11.928	37.502	-1.962	1.00	37.92
45	939	CG1	VAL	A	785	13.417	37.484	-2.236	1.00	35.87
	940	CG2	VAL	A	785	11.171	37.748	-3.264	1.00	33.21
	941	N	ARG	A	786	11.556	36.461	1.052	1.00	36.61
50	942	CA	ARG	A	786	12.091	36.278	2.406	1.00	38.66
	943	C	ARG	A	786	12.037	34.801	2.831	1.00	36.30
	944	O	ARG	A	786	13.008	34.249	3.362	1.00	38.29
55	945	CB	ARG	A	786	11.343	37.175	3.407	1.00	44.04
	946	CG	ARG	A	786	11.732	38.650	3.320	1.00	47.85
	947	CD	ARG	A	786	12.880	38.968	4.255	1.00	50.22
55	948	NE	ARG	A	786	12.397	39.082	5.635	1.00	62.62
	949	CZ	ARG	A	786	13.172	39.167	6.719	1.00	58.03
	950	NH1	ARG	A	786	14.494	39.134	6.609	1.00	61.23
	951	NH2	ARG	A	786	12.621	39.385	7.908	1.00	54.77

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5 952	N	MET	A	787	10.919	34.150	2.553	1.00	32.73
953	CA	MET	A	787	10.763	32.746	2.883	1.00	34.16
954	C	MET	A	787	11.733	31.878	2.066	1.00	38.91
10 955	O	MET	A	787	12.229	30.846	2.539	1.00	43.10
956	CB	MET	A	787	9.331	32.315	2.621	1.00	27.15
957	CG	MET	A	787	8.337	33.046	3.449	1.00	32.77
958	SD	MET	A	787	6.714	32.334	3.317	1.00	46.02
15 959	CE	MET	A	787	6.063	33.236	2.001	1.00	31.94
960	N	ARG	A	788	11.999	32.296	0.835	1.00	39.06
961	CA	ARG	A	788	12.902	31.570	-0.035	1.00	34.24
20 962	C	ARG	A	788	14.323	31.664	0.502	1.00	34.59
963	O	ARG	A	788	15.119	30.742	0.332	1.00	37.27
964	CB	ARG	A	788	12.790	32.122	-1.446	1.00	39.81
965	CG	ARG	A	788	13.263	31.196	-2.528	1.00	45.01
25 966	CD	ARG	A	788	12.846	31.727	-3.887	1.00	54.21
967	NE	ARG	A	788	13.605	32.913	-4.290	1.00	63.42
968	CZ	ARG	A	788	13.340	33.620	-5.386	1.00	68.54
30 969	NH1	ARG	A	788	12.329	33.261	-6.163	1.00	72.57
970	NH2	ARG	A	788	14.126	34.630	-5.752	1.00	72.25
971	N	HIS	A	789	14.636	32.759	1.191	1.00	40.92
972	CA	HIS	A	789	15.973	32.916	1.784	1.00	53.01
35 973	C	HIS	A	789	16.107	31.777	2.782	1.00	54.43
974	O	HIS	A	789	17.066	31.000	2.730	1.00	50.35
975	CB	HIS	A	789	16.114	34.232	2.575	1.00	64.44
40 976	CG	HIS	A	789	16.334	35.456	1.739	1.00	74.91
977	ND1	HIS	A	789	16.916	35.419	0.490	1.00	80.32
978	CD2	HIS	A	789	16.051	36.759	1.982	1.00	74.30
979	CE1	HIS	A	789	16.982	36.648	-0.001	1.00	78.33
45 980	NE2	HIS	A	789	16.465	37.481	0.886	1.00	74.90
981	N	LEU	A	790	15.112	31.700	3.674	1.00	56.83
982	CA	LEU	A	790	15.018	30.684	4.731	1.00	50.54
50 983	C	LEU	A	790	15.194	29.297	4.140	1.00	45.95
984	O	LEU	A	790	16.076	28.551	4.573	1.00	43.16
985	CB	LEU	A	790	13.660	30.757	5.427	1.00	47.65
986	CG	LEU	A	790	13.455	29.853	6.634	1.00	49.09
55 987	CD1	LEU	A	790	14.230	30.415	7.825	1.00	56.25
988	CD2	LEU	A	790	11.970	29.760	6.962	1.00	46.26

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	989	N	SER	A	791	14.388	28.963	3.130	38.77
	990	CA	SER	A	791	14.516	27.661	2.501	35.86
	991	C	SER	A	791	15.951	27.507	2.010	37.61
10	992	O	SER	A	791	16.533	26.432	2.127	42.51
	993	CB	SER	A	791	13.515	27.479	1.363	39.07
	994	OG	SER	A	791	13.974	28.090	0.177	55.38
	995	N	GLN	A	792	16.563	28.585	1.541	38.43
15	996	CA	GLN	A	792	17.938	28.481	1.086	43.65
	997	C	GLN	A	792	18.978	28.304	2.201	46.43
	998	O	GLN	A	792	20.049	27.761	1.951	53.03
20	999	CB	GLN	A	792	18.297	29.652	0.201	43.96
	1000	CG	GLN	A	792	17.455	29.723	-1.021	50.40
	1001	CD	GLN	A	792	17.516	31.082	-1.648	56.80
	1002	OE1	GLN	A	792	17.275	32.081	-0.975	59.46
25	1003	NE2	GLN	A	792	17.852	31.142	-2.938	56.24
	1004	N	GLU	A	793	18.684	28.734	3.424	46.80
	1005	CA	GLU	A	793	19.658	28.561	4.510	46.06
30	1006	C	GLU	A	793	19.852	27.078	4.787	40.74
	1007	O	GLU	A	793	20.972	26.632	5.000	41.28
	1008	CB	GLU	A	793	19.214	29.248	5.814	51.06
	1009	CG	GLU	A	793	18.949	30.772	5.734	67.15
35	1010	CD	GLU	A	793	20.212	31.644	5.762	74.35
	1011	OE1	GLU	A	793	21.328	31.098	5.703	72.15
	1012	OE2	GLU	A	793	20.083	32.894	5.837	83.11
40	1013	N	PHE	A	794	18.771	26.302	4.760	38.60
	1014	CA	PHE	A	794	18.862	24.866	5.031	36.65
	1015	C	PHE	A	794	19.960	24.277	4.206	40.69
45	1016	O	PHE	A	794	20.761	23.478	4.690	41.76
	1017	CB	PHE	A	794	17.562	24.160	4.686	32.29
	1018	CG	PHE	A	794	16.462	24.410	5.669	37.63
	1019	CD1	PHE	A	794	16.704	24.358	7.030	37.22
50	1020	CD2	PHE	A	794	15.173	24.718	5.229	43.04
	1021	CE1	PHE	A	794	15.665	24.605	7.945	35.06
	1022	CE2	PHE	A	794	14.126	24.969	6.140	37.46
55	1023	CZ	PHE	A	794	14.376	24.913	7.494	27.46
	1024	N	GLY	A	795	20.018	24.729	2.963	51.69
	1025	CA	GLY	A	795	21.033	24.260	2.040	57.61

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1026	C	GLY	A	795	22.440	24.695	2.391	1.00	58.51
	1027	O	GLY	A	795	23.338	23.850	2.481	1.00	54.63
	1028	N	TRP	A	796	22.625	25.994	2.624	1.00	56.85
10	1029	CA	TRP	A	796	23.942	26.504	2.944	1.00	61.47
	1030	C	TRP	A	796	24.433	25.986	4.301	1.00	59.21
	1031	O	TRP	A	796	25.614	25.649	4.469	1.00	55.17
15	1032	CB	TRP	A	796	23.966	28.039	2.770	1.00	77.04
	1033	CG	TRP	A	796	24.441	28.924	3.938	1.00	99.05
	1034	CD1	TRP	A	796	23.779	30.018	4.436	1.00	103.16
20	1035	CD2	TRP	A	796	25.693	28.847	4.686	1.00	107.94
	1036	NE1	TRP	A	796	24.528	30.622	5.430	1.00	107.43
	1037	CE2	TRP	A	796	25.701	29.929	5.606	1.00	109.90
25	1038	CE3	TRP	A	796	26.801	27.976	4.667	1.00	108.72
	1039	CZ2	TRP	A	796	26.778	30.157	6.503	1.00	110.69
	1040	CZ3	TRP	A	796	27.871	28.204	5.561	1.00	110.67
30	1041	CH2	TRP	A	796	27.845	29.286	6.462	1.00	111.09
	1042	N	LEU	A	797	23.500	25.779	5.221	1.00	56.75
	1043	CA	LEU	A	797	23.851	25.286	6.546	1.00	54.04
35	1044	C	LEU	A	797	24.012	23.767	6.640	1.00	56.56
	1045	O	LEU	A	797	24.629	23.277	7.587	1.00	62.03
	1046	CB	LEU	A	797	22.839	25.782	7.583	1.00	52.49
40	1047	CG	LEU	A	797	23.080	27.184	8.151	1.00	42.33
	1048	CD1	LEU	A	797	21.835	27.737	8.827	1.00	39.02
	1049	CD2	LEU	A	797	24.229	27.123	9.128	1.00	43.89
45	1050	N	GLN	A	798	23.462	23.020	5.684	1.00	53.42
	1051	CA	GLN	A	798	23.560	21.561	5.708	1.00	57.87
	1052	C	GLN	A	798	22.788	20.960	6.890	1.00	54.98
50	1053	O	GLN	A	798	23.268	20.039	7.571	1.00	53.85
	1054	CB	GLN	A	798	25.028	21.103	5.774	1.00	67.87
	1055	CG	GLN	A	798	25.773	21.088	4.438	1.00	83.30
55	1056	CD	GLN	A	798	27.115	20.345	4.507	1.00	91.19
	1057	OE1	GLN	A	798	27.910	20.564	5.428	1.00	96.98
	1058	NE2	GLN	A	798	27.368	19.463	3.532	1.00	87.09
55	1059	N	ILE	A	799	21.597	21.494	7.131	1.00	49.17
	1060	CA	ILE	A	799	20.728	21.040	8.219	1.00	45.76
	1061	C	ILE	A	799	20.348	19.545	8.071	1.00	47.10
	1062	O	ILE	A	799	19.766	19.135	7.059	1.00	40.12

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1063	CB	ILE	A	799	19.414	21.894	8.258	1.00	38.57
	1064	CG1	ILE	A	799	19.733	23.388	8.383	1.00	36.16
	1065	CG2	ILE	A	799	18.532	21.450	9.379	1.00	36.81
10	1066	CD1	ILE	A	799	20.686	23.691	9.480	1.00	27.19
	1067	N	THR	A	800	20.735	18.725	9.045	1.00	46.19
	1068	CA	THR	A	800	20.386	17.310	9.026	1.00	47.55
15	1069	C	THR	A	800	18.883	17.205	9.354	1.00	48.95
	1070	O	THR	A	800	18.345	18.013	10.125	1.00	55.00
	1071	CB	THR	A	800	21.222	16.474	10.060	1.00	47.29
20	1072	OG1	THR	A	800	20.773	16.729	11.396	1.00	53.15
	1073	CG2	THR	A	800	22.696	16.813	9.968	1.00	53.33
	1074	N	PRO	A	801	18.170	16.238	8.740	1.00	47.30
25	1075	CA	PRO	A	801	16.733	16.068	9.000	1.00	42.31
	1076	C	PRO	A	801	16.353	15.955	10.476	1.00	38.64
	1077	O	PRO	A	801	15.193	16.130	10.835	1.00	40.23
30	1078	CB	PRO	A	801	16.404	14.799	8.221	1.00	47.59
	1079	CG	PRO	A	801	17.285	14.951	7.007	1.00	46.66
	1080	CD	PRO	A	801	18.603	15.381	7.615	1.00	45.27
35	1081	N	GLN	A	802	17.351	15.682	11.310	1.00	41.68
	1082	CA	GLN	A	802	17.210	15.560	12.754	1.00	43.58
	1083	C	GLN	A	802	17.275	16.959	13.403	1.00	48.44
40	1084	O	GLN	A	802	16.505	17.266	14.329	1.00	49.81
	1085	CB	GLN	A	802	18.338	14.684	13.311	1.00	46.98
	1086	CG	GLN	A	802	18.321	13.250	12.830	1.00	46.45
45	1087	CD	GLN	A	802	18.685	13.116	11.373	1.00	48.73
	1088	OE1	GLN	A	802	19.827	13.413	10.968	1.00	53.22
	1089	NE2	GLN	A	802	17.727	12.666	10.566	1.00	43.12
50	1090	N	GLU	A	803	18.218	17.790	12.950	1.00	41.48
	1091	CA	GLU	A	803	18.322	19.142	13.483	1.00	32.56
	1092	C	GLU	A	803	17.034	19.841	13.133	1.00	34.21
55	1093	O	GLU	A	803	16.456	20.543	13.951	1.00	39.30
	1094	CB	GLU	A	803	19.485	19.869	12.879	1.00	27.56
	1095	CG	GLU	A	803	20.796	19.325	13.342	1.00	33.55
55	1096	CD	GLU	A	803	21.903	19.778	12.436	1.00	40.34
	1097	OE1	GLU	A	803	21.618	20.023	11.249	1.00	39.58
	1098	OE2	GLU	A	803	23.057	19.915	12.882	1.00	46.91
	1099	N	PHE	A	804	16.541	19.584	11.932	1.00	32.10

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1100	CA	PHE	A	804	15.286	20.166	11.519	1.00	26.58
	1101	C	PHE	A	804	14.157	19.876	12.497	1.00	29.08
	1102	O	PHE	A	804	13.528	20.793	13.024	1.00	38.23
10	1103	CB	PHE	A	804	14.872	19.663	10.142	1.00	24.46
	1104	CG	PHE	A	804	13.445	20.032	9.767	1.00	35.13
	1105	CD1	PHE	A	804	13.091	21.361	9.540	1.00	36.25
15	1106	CD2	PHE	A	804	12.468	19.048	9.617	1.00	38.14
	1107	CE1	PHE	A	804	11.795	21.712	9.164	1.00	27.83
	1108	CE2	PHE	A	804	11.163	19.385	9.238	1.00	39.32
20	1109	CZ	PHE	A	804	10.826	20.723	9.011	1.00	38.61
	1110	N	LEU	A	805	13.887	18.600	12.728	1.00	30.73
	1111 1	CA	LEU	A	805	12.784	18.215	13.586	1.00	28.43
25	1112	C	LEU	A	805	12.880	18.799	14.946	1.00	26.10
	1113	O	LEU	A	805	11.881	19.243	15.493	1.00	34.14
	1114	CB	LEU	A	805	12.648	16.702	13.661	1.00	34.10
30	1115	CG	LEU	A	805	12.000	16.079	12.423	1.00	43.20
	1116	CD1	LEU	A	805	12.046	14.617	12.600	1.00	36.94
	1117	CD2	LEU	A	805	10.549	16.523	12.252	1.00	44.97
35	1118	N	CYS	A	806	14.082	18.836	15.493	1.00	27.20
	1119	CA	CYS	A	806	14.250	19.396	16.831	1.00	39.83
	1120	C	CYS	A	806	13.904	20.894	16.843	1.00	41.37
40	1121	O	CYS	A	806	13.145	21.367	17.704	1.00	38.83
	1122	CB	CYS	A	806	15.669	19.143	17.341	1.00	43.31
	1123	SG	CYS	A	806	16.021	17.398	17.526	0.50	37.47
45	1124	N	MET	A	807	14.420	21.610	15.846	1.00	38.56
	1125	CA	MET	A	807	14.161	23.027	15.692	1.00	33.72
	1126	C	MET	A	807	12.662	23.301	15.488	1.00	31.70
50	1127	O	MET	A	807	12.093	24.168	16.148	1.00	37.83
	1128	CB	MET	A	807	14.973	23.589	14.519	1.00	37.50
	1129	CG	MET	A	807	16.474	23.539	14.740	1.00	38.94
55	1130	SD	MET	A	807	17.486	24.563	13.596	1.00	42.84
	1131	CE	MET	A	807	17.165	23.799	12.065	1.00	49.58
	1132	N	LYS	A	808	12.006	22.545	14.617	1.00	27.59
55	1133	CA	LYS	A	808	10.597	22.787	14.378	1.00	27.15
	1134	C	LYS	A	808	9.841	22.681	15.686	1.00	29.83
	1135	O	LYS	A	808	8.954	23.486	15.952	1.00	35.67
	1136	CB	LYS	A	808	10.029	21.837	13.313	1.00	24.49

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1137	CG	LYS	A	808	8.598	22.158	12.811 1	1.00	23.62
	1138	CD	LYS	A	808	8.148	21.143	11.740	1.00	24.64
	1139	CE	LYS	A	808	7.157	20.101	12.280	1.00	29.39
10	1140	NZ	LYS	A	808	5.683	20.529	12.198	1.00	36.92
	1141	N	ALA	A	809	10.220	21.727	16.530	1.00	32.53
	1142	CA	ALA	A	809	9.553	21.557	17.826	1.00	38.51
15	1143	C	ALA	A	809	9.786	22.766	18.749	1.00	43.27
	1144	O	ALA	A	809	8.844	23.305	19.346	1.00	43.55
	1145	CB	ALA	A	809	10.029	20.295	18.501	1.00	25.72
20	1146	N	LEU	A	810	11.042	23.193	18.836	1.00	41.18
	1147	CA	LEU	A	810	11.460	24.340	19.651	1.00	40.05
	1148	C	LEU	A	810	10.732	25.626	19.269	1.00	38.85
25	1149	O	LEU	A	810	10.445	26.460	20.134	1.00	38.70
	1150	CB	LEU	A	810	12.961	24.534	19.502	1.00	39.64
	1151	CG	LEU	A	810	13.779	25.313	20.524	1.00	43.39
30	1152	CD1	LEU	A	810	13.361	24.959	21.942	1.00	41.58
	1153	CD2	LEU	A	810	15.256	24.981	20.284	1.00	34.95
	1154	N	LEU	A	811	10.409	25.763	17.982	1.00	31.82
35	1155	CA	LEU	A	811	9.683	26.923	17.489	1.00	34.47
	1156	C	LEU	A	811	8.359	27.093	18.200	1.00	35.94
	1157	O	LEU	A	811	7.918	28.219	18.435	1.00	47.05
40	1158	CB	LEU	A	811	9.384	26.811	15.988	1.00	33.79
	1159	CG	LEU	A	811	10.309	27.474	14.973	1.00	28.95
	1160	CD1	LEU	A	811	9.523	27.595	13.709	1.00	30.30
45	1161	CD2	LEU	A	811	10.767	28.875	15.444	1.00	20.35
	1162	N	LEU	A	812	7.713	25.978	18.527	1.00	31.68
	1163	CA	LEU	A	812	6.418	26.032	19.190	1.00	30.90
50	1164	C	LEU	A	812	6.459	26.850	20.469	1.00	29.57
	1165	O	LEU	A	812	5.476	27.486	20.836	1.00	35.81
	1166	CB	LEU	A	812	5.934	24.622	19.511	1.00	29.23
55	1167	CG	LEU	A	812	4.600	24.544	20.281	1.00	34.64
	1168	CD1	LEU	A	812	3.428	25.002	19.417	1.00	30.86
	1169	CD2	LEU	A	812	4.355	23.144	20.738	1.00	31.58
55	1170	N	PHE	A	813	7.604	26.788	21.144	1.00	32.36
	1171	CA	PHE	A	813	7.862	27.480	22.405	1.00	36.84
	1172	C	PHE	A	813	8.709	28.693	22.180	1.00	36.98
	1173	O	PHE	A	813	9.584	28.983	22.996	1.00	34.78

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1174	CB	PHE	A	813	8.669	26.585	23.335	1.00	39.81
	1175	CG	PHE	A	813	8.119	25.242	23.454	1.00	42.06
	1176	CD1	PHE	A	813	6.837	25.057	23.960	1.00	40.53
10	1177	CD2	PHE	A	813	8.826	24.156	22.984	1.00	43.44
	1178	CE1	PHE	A	813	6.255	23.794	23.990	1.00	49.40
	1179	CE2	PHE	A	813	8.259	22.884	23.006	1.00	48.76
15	1180	CZ	PHE	A	813	6.966	22.698	23.510	1.00	49.26
	1181	N	SER	A	814	8.488	29.380	21.071	1.00	39.85
	1182	CA	SER	A	814	9.284	30.547	20.748	1.00	40.33
20	1183	C	SER	A	814	8.531	31.858	20.778	1.00	34.59
	1184	O	SER	A	814	9.125	32.897	20.612	1.00	39.81
	1185	CB	SER	A	814	9.938	30.364	19.374	1.00	45.33
25	1186	OG	SER	A	814	11.096	29.544	19.469	1.00	51.73
	1187	N	ILE	A	815	7.242	31.838	21.040	1.00	38.17
	1188	CA	ILE	A	815	6.508	33.083	21.033	1.00	46.03
30	1189	C	ILE	A	815	5.456	33.076	22.149	1.00	46.20
	1190	O	ILE	A	815	4.526	32.260	22.112	1.00	45.64
	1191	CB	ILE	A	815	5.937	33.329	19.597	1.00	49.44
35	1192	CG1	ILE	A	815	4.943	34.477	19.593	1.00	50.62
	1193	CG2	ILE	A	815	5.401	32.041	18.971	1.00	50.44
	1194	CD1	ILE	A	815	5.406	35.592	18.748	1.00	55.65
40	1195	N	ILE	A	816	5.645	33.950	23.152	1.00	47.67
	1196	CA	ILE	A	816	4.762	34.056	24.344	1.00	46.12
	1197	C	ILE	A	816	4.302	35.482	24.731	1.00	42.20
45	1198	O	ILE	A	816	5.002	36.460	24.436	1.00	43.23
	1199	CB	ILE	A	816	5.446	33.417	25.609	1.00	50.07
	1200	CG1	ILE	A	816	6.701	34.194	26.018	1.00	49.09
50	1201	CG2	ILE	A	816	5.819	31.970	25.326	1.00	52.85
	1202	CD1	ILE	A	816	7.442	33.578	27.204	1.00	37.43
	1203	N	PRO	A	817	3.123	35.618	25.402	1.00	37.07
55	1204	CA	PRO	A	817	2.619	36.933	25.811	1.00	40.94
	1205	C	PRO	A	817	3.702	37.599	26.659	1.00	49.75
	1206	O	PRO	A	817	4.595	36.891	27.163	1.00	47.60
	1207	CB	PRO	A	817	1.396	36.581	26.662	1.00	27.66
	1208	CG	PRO	A	817	0.902	35.368	26.063	1.00	28.99
	1209	CD	PRO	A	817	2.186	34.579	25.855	1.00	33.43
	1210	N	VAL	A	818	3.663	38.933	26.798	1.00	57.41

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1211	CA	VAL	A	818	4.690	39.631	27.592	1.00	58.97
	1212	C	VAL	A	818	4.728	39.410	29.124	1.00	59.31
	1213	O	VAL	A	818	5.801	39.574	29.720	1.00	63.79
10	1214	CB	VAL	A	818	4.893	41.127	27.206	1.00	54.46
	1215	CG1	VAL	A	818	5.738	41.211	25.950	1.00	49.94
	1216	CG2	VAL	A	818	3.575	41.824	27.009	1.00	53.66
15	1217	N	ASP	A	819	3.607	39.061	29.769	1.00	56.35
	1218	CA	ASP	A	819	3.654	38.741	31.212	1.00	61.78
	1219	C	ASP	A	819	4.167	37.302	31.212	1.00	63.93
20	1220	O	ASP	A	819	5.322	36.998	31.566	1.00	69.29
	1221	CB	ASP	A	819	2.270	38.746	31.869	1.00	60.71
	1222	CG	ASP	A	819	1.174	39.031	30.888	1.00	71.79
25	1223	OD1	ASP	A	819	0.947	40.218	30.600	1.00	78.23
	1224	OD2	ASP	A	819	0.577	38.069	30.373	1.00	78.87
	1225	N	GLY	A	820	3.296	36.419	30.758	1.00	57.92
30	1226	CA	GLY	A	820	3.652	35.034	30.672	1.00	46.58
	1227	C	GLY	A	820	2.369	34.304	30.440	1.00	45.74
	1228	O	GLY	A	820	1.293	34.894	30.200	1.00	40.14
35	1229	N	LEU	A	821	2.497	32.995	30.500	1.00	46.98
	1230	CA	LEU	A	821	1.378	32.105	30.327	1.00	47.93
	1231	C	LEU	A	821	0.787	31.902	31.733	1.00	47.05
40	1232	O	LEU	A	821	1.456	32.188	32.737	1.00	45.88
	1233	CB	LEU	A	821	1.905	30.808	29.708	1.00	54.39
	1234	CG	LEU	A	821	2.560	31.017	28.336	1.00	50.67
45	1235	CD1	LEU	A	821	3.858	30.259	28.235	1.00	43.32
	1236	CD2	LEU	A	821	1.602	30.622	27.240	1.00	46.90
	1237	N	LYS	A	822	-0.437	31.393	31.820	1.00	48.17
50	1238	CA	LYS	A	822	-1.103	31.181	33.105	1.00	52.88
	1239	C	LYS	A	822	-0.449	30.065	33.935	1.00	59.84
	1240	O	LYS	A	822	-1.111	29.361	34.709	1.00	62.81
55	1241	CB	LYS	A	822	-2.609	30.951	32.880	1.00	56.87
	1242	CG	LYS	A	822	-3.321	32.193	32.288	1.00	65.23
	1243	CD	LYS	A	822	-4.729	31.923	31.719	1.00	63.38
55	1244	CE	LYS	A	822	-5.371	33.194	31.088	1.00	65.28
	1245	NZ	LYS	A	822	-4.534	33.875	30.032	1.00	59.84
	1246	N	ASN	A	823	0.862	29.930	33.744	1.00	62.47
	1247	CA	ASN	A	823	1.739	28.988	34.419	1.00	60.37

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1248	C	ASN	A	823	3.025	28.904	33.616	1.00	58.03
1249	O	ASN	A	823	3.364	27.879	33.017	1.00	50.60
1250	CB	ASN	A	823	1.138	27.611	34.544	1.00	65.57
1251	CG	ASN	A	823	2.094	26.649	35.178	1.00	75.73
1252	OD1	ASN	A	823	3.101	27.051	35.811	1.00	68.88
1253	ND2	ASN	A	823	1.830	25.367	34.986	1.00	81.03
1254	N	GLN	A	824	3.743	30.012	33.631	1.00	59.10
1255	CA	GLN	A	824	4.993	30.158	32.914	1.00	56.38
1256	C	GLN	A	824	6.069	29.145	33.329	1.00	54.52
1257	O	GLN	A	824	6.826	28.677	32.483	1.00	53.91
1258	CB	GLN	A	824	5.485	31.592	33.129	1.00	56.68
1259	CG	GLN	A	824	6.761	31.972	32.412	1.00	54.92
1260	CD	GLN	A	824	6.532	32.329	30.976	1.00	59.81
1261	OE1	GLN	A	824	5.462	32.833	30.602	1.00	57.91
1262	NE2	GLN	A	824	7.533	32.078	30.150	1.00	62.36
1263	N	LYS	A	825	6.099	28.777	34.613	1.00	55.18
1264	CA	LYS	A	825	7.098	27.841	35.160	1.00	53.31
1265	C	LYS	A	825	7.351	26.550	34.357	1.00	46.62
1266	O	LYS	A	825	8.497	26.236	34.015	1.00	40.85
1267	CB	LYS	A	825	6.769	27.515	36.626	1.00	57.76
1268	CG	LYS	A	825	7.128	28.634	37.617	1.00	64.19
1269	CD	LYS	A	825	6.432	28.463	38.979	1.00	77.45
1270	CE	LYS	A	825	7.122	29.254	40.125	1.00	86.97
1271	NZ	LYS	A	825	7.186	30.763	40.023	1.00	89.42
1272	N	PHE	A	826	6.285	25.811	34.053	1.00	46.35
1273	CA	PHE	A	826	6.399	24.562	33.288	1.00	47.42
1274	C	PHE	A	826	6.892	24.863	31.853	1.00	48.67
1275	O	PHE	A	826	7.847	24.243	31.395	1.00	48.05
1276	CB	PHE	A	826	5.063	23.774	33.273	1.00	43.87
1277	CG	PHE	A	826	4.588	23.295	34.653	1.00	56.48
1278	CD1	PHE	A	826	5.443	23.288	35.770	1.00	62.15
1279	CD2	PHE	A	826	3.273	22.832	34.831	1.00	60.89
1280	CE1	PHE	A	826	4.994	22.827	37.040	1.00	53.25
1281	CE2	PHE	A	826	2.813	22.367	36.097	1.00	53.93
1282	CZ	PHE	A	826	3.681	22.368	37.193	1.00	51.47
1283	N	PHE	A	827	6.272	25.835	31.168	1.00	44.70
1284	CA	PHE	A	827	6.670	26.234	29.800	1.00	40.53

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1285	C	PHE	A	827	8.181	26.414	29.746	1.00	37.37
	1286	O	PHE	A	827	8.848	25.934	28.835	1.00	35.40
	1287	CB	PHE	A	827	5.964	27.558	29.375	1.00	35.40
10	1288	CG	PHE	A	827	6.497	28.177	28.070	1.00	31.04
	1289	CD1	PHE	A	827	7.750	28.793	28.018	1.00	32.73
	1290	CD2	PHE	A	827	5.742	28.125	26.900	1.00	34.40
15	1291	CE1	PHE	A	827	8.239	29.331	26.834	1.00	34.03
	1292	CE2	PHE	A	827	6.225	28.664	25.705	1.00	26.27
	1293	CZ	PHE	A	827	7.472	29.265	25.676	1.00	30.82
20	1294	N	ASP	A	828	8.705	27.105	30.745	1.00	42.94
	1295	CA	ASP	A	828	10.120	27.388	30.829	1.00	49.10
	1296	C	ASP	A	828	10.933	26.130	31.071	1.00	49.16
25	1297	O	ASP	A	828	12.107	26.056	30.681	1.00	48.64
	1298	CB	ASP	A	828	10.371	28.459	31.899	1.00	53.78
	1299	CG	ASP	A	828	9.730	29.810	31.539	1.00	65.91
30	1300	OD1	ASP	A	828	9.610	30.121	30.329	1.00	69.82
	1301	OD2	ASP	A	828	9.357	30.576	32.461	1.00	63.94
	1302	N	GLU	A	829	10.313	25.138	31.703	1.00	49.55
35	1303	CA	GLU	A	829	10.997	23.875	31.941	1.00	49.00
	1304	C	GLU	A	829	10.952	23.103	30.622	1.00	37.58
	1305	O	GLU	A	829	11.969	22.573	30.177	1.00	35.86
40	1306	CB	GLU	A	829	10.350	23.073	33.076	1.00	61.68
	1307	CG	GLU	A	829	11.366	22.268	33.925	1.00	81.07
	1308	CD	GLU	A	829	10.939	20.814	34.222	1.00	92.42
45	1309	OE1	GLU	A	829	9.952	20.603	34.969	1.00	97.07
	1310	OE2	GLU	A	829	11.619	19.881	33.727	1.00	91.99
	1311	N	LEU	A	830	9.794	23.102	29.962	1.00	33.30
50	1312	CA	LEU	A	830	9.626	22.436	28.661	1.00	37.63
	1313	C	LEU	A	830	10.621	23.003	27.673	1.00	41.33
	1314	O	LEU	A	830	11.366	22.261	27.031	1.00	46.84
55	1315	CB	LEU	A	830	8.240	22.701	28.083	1.00	30.37
	1316	CG	LEU	A	830	7.257	21.551	28.118	1.00	39.95
	1317	CD1	LEU	A	830	6.108	21.877	27.212	1.00	34.14
55	1318	CD2	LEU	A	830	7.951	20.268	27.671	1.00	49.69
	1319	N	ARG	A	831	10.621	24.333	27.566	1.00	44.13
	1320	CA	ARG	A	831	11.504	25.048	26.658	1.00	40.24
	1321	C	ARG	A	831	12.977	24.673	26.862	1.00	37.21

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1322	O	ARG	A	831	13.690	24.354	25.901	1.00	37.75
1323	CB	ARG	A	831	11.285	26.566	26.765	1.00	34.87
1324	CG	ARG	A	831	12.179	27.322	25.816	1.00	34.44
1325	CD	ARG	A	831	11.915	28.804	25.731	1.00	38.71
1326	NE	ARG	A	831	13.020	29.423	25.006	1.00	39.34
1327	CZ	ARG	A	831	13.073	29.573	23.682	1.00	44.99
1328	NH1	ARG	A	831	12.060	29.164	22.926	1.00	40.07
1329	NH2	ARG	A	831	14.178	30.050	23.104	1.00	41.88
1330	N	MET	A	832	13.411	24.625	28.116	1.00	38.65
1331	CA	MET	A	832	14.799	24.281	28.440	1.00	43.09
1332	C	MET	A	832	15.239	22.880	27.996	1.00	44.84
1333	O	MET	A	832	16.400	22.662	27.602	1.00	43.33
1334	CB	MET	A	832	15.065	24.409	29.941	1.00	41.77
1335	CG	MET	A	832	16.486	23.967	30.274	1.00	50.47
1336	SD	MET	A	832	16.856	23.608	31.997	1.00	61.59
1337	CE	MET	A	832	15.233	23.187	32.715	1.00	51.34
1338	N	ASN	A	833	14.339	21.914	28.141	1.00	46.14
1339	CA	ASN	A	833	14.661	20.552	27.754	1.00	44.12
1340	C	ASN	A	833	14.756	20.387	26.255	1.00	40.57
1341	O	ASN	A	833	15.670	19.729	25.766	1.00	45.06
1342	CB	ASN	A	833	13.689	19.580	28.379	1.00	47.22
1343	CG	ASN	A	833	14.098	19.202	29.782	1.00	44.35
1344	OD1	ASN	A	833	15.262	18.849	30.041	1.00	53.06
1345	ND2	ASN	A	833	13.161	19.299	30.705	1.00	42.24
1346	N	TYR	A	834	13.866	21.048	25.523	1.00	35.70
1347	CA	TYR	A	834	13.923	21.006	24.074	1.00	36.60
1348	C	TYR	A	834	15.260	21.582	23.589	1.00	35.58
1349	O	TYR	A	834	15.891	21.044	22.670	1.00	39.23
1350	CB	TYR	A	834	12.723	21.729	23.473	1.00	33.03
1351	CG	TYR	A	834	11.480	20.849	23.446	1.00	39.21
1352	CD1	TYR	A	834	10.724	20.630	24.597	1.00	41.70
1353	CD2	TYR	A	834	11.085	20.196	22.274	1.00	38.14
1354	CE1	TYR	A	834	9.598	19.774	24.587	1.00	44.38
1355	CE2	TYR	A	834	9.959	19.337	22.255	1.00	42.60
1356	CZ	TYR	A	834	9.229	19.132	23.416	1.00	42.12
1357	OH	TYR	A	834	8.164	18.264	23.404	1.00	38.82
1358	N	ILE	A	835	15.754	22.607	24.275	1.00	37.68

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1359	CA	ILE	A	835	17.042	23.197	23.901	1.00	42.31
	1360	C	ILE	A	835	18.103	22.133	24.060	1.00	42.75
	1361	O	ILE	A	835	18.995	21.997	23.217	1.00	45.95
10	1362	CB	ILE	A	835	17.408	24.417	24.782	1.00	37.10
	1363	CG1	ILE	A	835	16.357	25.512	24.558	1.00	41.30
	1364	CG2	ILE	A	835	18.832	24.912	24.457	1.00	29.58
	1365	CD1	ILE	A	835	16.610	26.802	25.286	1.00	39.55
15	1366	N	LYS	A	836	17.980	21.373	25.144	1.00	44.22
	1367	CA	LYS	A	836	18.925	20.313	25.442	1.00	44.77
	1368	C	LYS	A	836	18.846	19.252	24.363	1.00	41.28
20	1369	O	LYS	A	836	19.866	18.780	23.914	1.00	46.84
	1370	CB	LYS	A	836	18.655	19.694	26.813	1.00	46.26
	1371	CG	LYS	A	836	19.116	20.512	28.011	1.00	49.87
25	1372	CD	LYS	A	836	18.609	19.834	29.274	0.00	50.55
	1373	CE	LYS	A	836	19.311	20.321	30.524	0.00	51.77
	1374	NZ	LYS	A	836	18.709	19.697	31.735	0.00	52.70
	1375	N	GLU	A	837	17.655	18.928	23.883	1.00	40.62
30	1376	CA	GLU	A	837	17.543	17.899	22.851	1.00	44.21
	1377	C	GLU	A	837	18.253	18.344	21.603	1.00	43.91
	1378	O	GLU	A	837	18.902	17.549	20.922	1.00	49.11
35	1379	CB	GLU	A	837	16.077	17.573	22.516	1.00	43.88
	1380	CG	GLU	A	837	15.226	17.032	23.675	1.00	44.03
	1381	CD	GLU	A	837	15.937	15.978	24.534	1.00	50.34
	1382	OE1	GLU	A	837	16.915	15.332	24.076	1.00	45.21
40	1383	OE2	GLU	A	837	15.512	15.804	25.696	1.00	56.07
	1384	N	LEU	A	838	18.113	19.627	21.305	1.00	44.87
45	1385	CA	LEU	A	838	18.739	20.218	20.139	1.00	43.87
	1386	C	LEU	A	838	20.244	20.120	20.285	1.00	42.53
	1387	O	LEU	A	838	20.949	19.835	19.332	1.00	42.95
	1388	CB	LEU	A	838	18.324	21.675	20.019	1.00	42.66
	1389	CG	LEU	A	838	19.051	22.463	18.932	1.00	44.98
50	1390	CD1	LEU	A	838	18.810	21.814	17.567	1.00	39.69
	1391	CD2	LEU	A	838	18.571	23.909	18.964	1.00	37.64
	1392	N	ASP	A	839	20.713	20.346	21.501	1.00	44.58
55	1393	CA	ASP	A	839	22.129	20.286	21.844	1.00	52.02
	1394	C	ASP	A	839	22.630	18.829	21.696	1.00	57.30
	1395	O	ASP	A	839	23.750	18.569	21.224	1.00	54.16

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1396	CB	ASP	A	839	22.262	20.760	23.305	1.00	59.66
	1397	CG	ASP	A	839	23.673	21.234	23.674	1.00	66.70
	1398	OD1	ASP	A	839	24.584	21.284	22.812	1.00	65.99
	1399	OD2	ASP	A	839	23.850	21.598	24.860	1.00	68.25
10	1400	N	ARG	A	840	21.768	17.884	22.081	1.00	62.29
	1401	CA	ARG	A	840	22.065	16.453	22.022	1.00	62.05
	1402	C	ARG	A	840	22.280	16.022	20.591	1.00	60.23
15	1403	O	ARG	A	840	23.331	15.468	20.268	1.00	57.37
	1404	CB	ARG	A	840	20.927	15.623	22.643	1.00	61.97
	1405	CG	ARG	A	840	21.035	14.114	22.407	1.00	62.90
	1406	CD	ARG	A	840	20.219	13.320	23.422	1.00	62.88
20	1407	NE	ARG	A	840	20.676	13.542	24.799	1.00	67.96
	1408	CZ	ARG	A	840	19.875	13.676	25.861	1.00	65.20
	1409	NH1	ARG	A	840	18.550	13.618	25.718	1.00	60.29
25	1410	NH2	ARG	A	840	20.404	13.889	27.066	1.00	61.82
	1411	N	ILE	A	841	21.298	16.311	19.739	1.00	57.25
	1412	CA	ILE	A	841	21.344	15.956	18.325	1.00	64.29
30	1413	C	ILE	A	841	22.494	16.602	17.508	1.00	71.86
	1414	O	ILE	A	841	22.706	16.276	16.327	1.00	78.18
	1415	CB	ILE	A	841	19.998	16.261	17.674	1.00	66.05
	1416	CG1	ILE	A	841	19.813	17.765	17.505	1.00	60.52
35	1417	CG2	ILE	A	841	18.887	15.730	18.567	1.00	69.45
	1418	CD1	ILE	A	841	18.835	18.115	16.439	1.00	55.24
	1419	N	ILE	A	842	23.210	17.541	18.127	1.00	74.71
40	1420	CA	ILE	A	842	24.354	18.208	17.489	1.00	72.84
	1421	C	ILE	A	842	25.643	17.430	17.845	1.00	76.76
	1422	O	ILE	A	842	26.431	17.080	16.952	1.00	76.88
	1423	CB	ILE	A	842	24.507	19.684	17.990	1.00	62.10
45	1424	CG1	ILE	A	842	23.312	20.522	17.569	1.00	54.67
	1425	CG2	ILE	A	842	25.769	20.303	17.439	1.00	59.08
	1426	CD1	ILE	A	842	23.101	20.519	16.109	1.00	56.78
50	1427	N	ALA	A	843	25.819	17.166	19.152	1.00	82.38
	1428	CA	ALA	A	843	26.979	16.461	19.733	1.00	81.09
	1429	C	ALA	A	843	26.960	14.955	19.524	1.00	79.83
	1430	O	ALA	A	843	27.924	14.260	19.838	1.00	79.34
55	1431	CB	ALA	A	843	27.076	16.768	21.247	1.00	73.81
	1432	N	CYS	A	844	25.872	14.469	18.947	1.00	80.33

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1433	CA	CYS	A	844	25.657	13.052	18.721	1.00	80.34
	1434	C	CYS	A	844	25.771	12.645	17.215	1.00	84.98
	1435	O	CYS	A	844	25.056	11.750	16.759	1.00	90.65
10	1436	CB	CYS	A	844	24.269	12.717	19.315	1.00	80.98
	1437	SG	CYS	A	844	24.002	11.110	20.120	1.00	93.38
	1438	N	LYS	A	845	26.665	13.302	16.460	1.00	86.19
15	1439	CA	LYS	A	845	26.917	13.002	15.026	1.00	83.63
	1440	C	LYS	A	845	28.420	13.101	14.620	1.00	90.32
	1441	O	LYS	A	845	29.110	12.079	14.517	1.00	87.60
20	1442	CB	LYS	A	845	26.063	13.874	14.087	1.00	72.76
	1443	CG	LYS	A	845	24.727	13.263	13.735	1.00	66.51
	1444	CD	LYS	A	845	23.998	14.104	12.702	0.00	63.58
25	1445	CE	LYS	A	845	24.644	14.005	11.326	0.00	60.54
	1446	NZ	LYS	A	845	23.795	13.251	10.351	0.00	57.84
	1447	N	ARG	A	846	28.929	14.316	14.384	1.00	97.68
30	1448	CA	ARG	A	846	30.336	14.489	13.998	1.00	99.68
	1449	C	ARG	A	846	31.289	15.076	15.097	1.00	104.16
	1450	O	ARG	A	846	31.315	14.556	16.229	1.00	101.78
35	1451	CB	ARG	A	846	30.442	15.246	12.671	1.00	94.46
	1452	CG	ARG	A	846	31.702	14.917	11.839	1.00	92.16
	1453	CD	ARG	A	846	31.538	13.643	10.999	1.00	87.99
40	1454	NE	ARG	A	846	32.671	12.718	11.128	1.00	86.09
	1455	CZ	ARG	A	846	32.667	11.463	10.675	1.00	85.82
	1456	NH1	ARG	A	846	31.583	10.985	10.058	1.00	79.74
45	1457	NH2	ARG	A	846	33.720	10.666	10.891	1.00	82.90
	1458	N	LYS	A	847	32.040	16.139	14.736	1.00	109.20
	1459	CA	LYS	A	847	33.061	16.820	15.585	1.00	108.66
50	1460	C	LYS	A	847	32.769	17.424	16.961	1.00	113.81
	1461	O	LYS	A	847	31.596	17.569	17.368	1.00	118.99
	1462	CB	LYS	A	847	33.760	17.897	14.758	0.00	98.30
55	1463	CG	LYS	A	847	34.514	17.383	13.563	0.00	85.34
	1464	CD	LYS	A	847	35.150	18.542	12.840	0.00	73.33
	1465	CE	LYS	A	847	35.928	18.073	11.641	0.00	64.16
55	1466	NZ	LYS	A	847	36.604	19.219	10.996	0.00	56.55
	1467	N	ASN	A	848	33.860	17.821	17.636	1.00	115.89
	1468	CA	ASN	A	848	33.904	18.449	18.991	1.00	116.39
	1469	C	ASN	A	848	35.379	18.906	19.266	1.00	119.41

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1470	O	ASN	A	848	36.305	18.286	18.735	1.00	122.42
1471	CB	ASN	A	848	33.392	17.448	20.089	1.00	106.55
1472	CG	ASN	A	848	33.984	16.032	19.955	1.00	99.70
1473	OD1	ASN	A	848	35.078	15.825	19.426	1.00	96.25
1474	ND2	ASN	A	848	33.240	15.046	20.457	1.00	89.90
1475	N	PRO	A	849	35.622	20.019	20.031	1.00	119.93
1476	CA	PRO	A	849	34.808	21.031	20.742	1.00	119.46
1477	C	PRO	A	849	34.292	22.298	20.008	1.00	118.74
1478	O	PRO	A	849	33.082	22.562	20.025	1.00	121.98
1479	CB	PRO	A	849	35.725	21.422	21.914	1.00	118.16
1480	CG	PRO	A	849	37.063	21.454	21.259	1.00	118.96
1481	CD	PRO	A	849	37.039	20.160	20.430	1.00	120.61
1482	N	THR	A	850	35.178	23.098	19.399	1.00	113.94
1483	CA	THR	A	850	34.738	24.330	18.701	1.00	107.06
1484	C	THR	A	850	33.693	24.100	17.584	1.00	103.74
1485	O	THR	A	850	32.820	24.944	17.372	1.00	104.75
1486	CB	THR	A	850	35.931	25.182	18.134	1.00	105.27
1487	OG1	THR	A	850	36.538	24.500	17.025	1.00	104.75
1488	CG2	THR	A	850	36.976	25.482	19.222	1.00	99.79
1489	N	SER	A	851	33.788	22.949	16.909	1.00	98.29
1490	CA	SER	A	851	32.885	22.562	15.810	1.00	93.63
1491	C	SER	A	851	31.374	22.559	16.173	1.00	89.97
1492	O	SER	A	851	30.553	23.123	15.429	1.00	85.73
1493	CB	SER	A	851	33.319	21.185	15.262	1.00	93.65
1494	OG	SER	A	851	32.729	20.888	14.012	1.00	96.10
1495	N	CYS	A	852	31.000	21.964	17.311	1.00	87.36
1496	CA	CYS	A	852	29.587	21.932	17.706	1.00	85.60
1497	C	CYS	A	852	29.128	23.167	18.541	1.00	85.71
1498	O	CYS	A	852	27.929	23.468	18.592	1.00	81.46
1499	CB	CYS	A	852	29.260	20.605	18.409	1.00	85.66
1500	SG	CYS	A	852	29.511	20.548	20.196	1.00	92.38
1501	N	SER	A	853	30.071	23.873	19.184	1.00	88.63
1502	CA	SER	A	853	29.760	25.085	19.970	1.00	85.42
1503	C	SER	A	853	29.261	26.147	18.970	1.00	81.80
1504	O	SER	A	853	28.320	26.914	19.260	1.00	75.88
1505	CB	SER	A	853	31.015	25.615	20.702	1.00	83.41
1506	OG	SER	A	853	31.524	24.733	21.692	1.00	75.95

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1507	N	ARG	A	854	29.929	26.190	17.806	1.00	77.44
	1508	CA	ARG	A	854	29.586	27.108	16.721	1.00	75.23
	1509	C	ARG	A	854	28.428	26.555	15.903	1.00	68.44
10	1510	O	ARG	A	854	27.614	27.325	15.381	1.00	64.21
	1511	CB	ARG	A	854	30.803	27.423	15.831	1.00	83.31
	1512	CG	ARG	A	854	31.492	26.211	15.215	1.00	95.75
15	1513	CD	ARG	A	854	32.915	26.540	14.706	1.00	105.49
	1514	NE	ARG	A	854	32.927	27.070	13.344	1.00	111.61
	1515	CZ	ARG	A	854	33.255	28.318	13.014	1.00	107.74
20	1516	NH1	ARG	A	854	33.614	29.182	13.963	1.00	108.73
	1517	NH2	ARG	A	854	33.171	28.704	11.740	1.00	100.08
	1518	N	ARG	A	855	28.341	25.228	15.801	1.00	62.47
25	1519	CA	ARG	A	855	27.229	24.606	15.087	1.00	56.87
	1520	C	ARG	A	855	25.922	24.945	15.831	1.00	55.34
	1521	O	ARG	A	855	24.861	25.054	15.206	1.00	61.05
30	1522	CB	ARG	A	855	27.423	23.085	14.974	1.00	53.03
	1523	CG	ARG	A	855	26.247	22.321	14.341	1.00	51.39
	1524	CD	ARG	A	855	25.983	22.707	12.891	1.00	55.10
35	1525	NE	ARG	A	855	24.943	21.899	12.233	1.00	54.36
	1526	CZ	ARG	A	855	24.745	21.858	10.911	1.00	55.00
	1527	NH1	ARG	A	855	25.517	22.579	10.110	1.00	52.83
40	1528	NH2	ARG	A	855	23.796	21.094	10.384	1.00	48.85
	1529	N	PHE	A	856	26.003	25.152	17.152	1.00	52.54
	1530	CA	PHE	A	856	24.817	25.508	17.962	1.00	49.53
45	1531	C	PHE	A	856	24.438	26.974	17.738	1.00	48.70
	1532	O	PHE	A	856	23.254	27.326	17.597	1.00	45.42
	1533	CB	PHE	A	856	25.066	25.270	19.457	1.00	46.16
50	1534	CG	PHE	A	856	23.852	25.527	20.319	1.00	46.93
	1535	CD1	PHE	A	856	22.699	24.751	20.170	1.00	47.04
	1536	CD2	PHE	A	856	23.845	26.549	21.259	1.00	41.32
55	1537	CE1	PHE	A	856	21.547	24.986	20.949	1.00	46.91
	1538	CE2	PHE	A	856	22.711	26.785	22.033	1.00	45.75
	1539	CZ	PHE	A	856	21.553	25.999	21.877	1.00	42.35
55	1540	N	TYR	A	857	25.461	27.822	17.725	1.00	47.67
	1541	CA	TYR	A	857	25.283	29.238	17.487	1.00	47.32
	1542	C	TYR	A	857	24.503	29.373	16.181	1.00	44.87
	1543	O	TYR	A	857	23.404	29.945	16.159	1.00	42.27

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1544	CB	TYR	A	857	26.667	29.901	17.407	1.00	50.61
	1545	CG	TYR	A	857	26.684	31.282	16.807	1.00	54.67
	1546	CD1	TYR	A	857	26.450	32.422	17.593	1.00	59.56
10	1547	CD2	TYR	A	857	26.935	31.454	15.442	1.00	54.77
	1548	CE1	TYR	A	857	26.469	33.719	17.022	1.00	58.68
	1549	CE2	TYR	A	857	26.953	32.728	14.860	1.00	58.39
	1550	CZ	TYR	A	857	26.720	33.855	15.647	1.00	61.97
15	1551	OH	TYR	A	857	26.725	35.091	15.035	1.00	56.70
	1552	N	GLN	A	858	25.006	28.706	15.141	1.00	43.56
	1553	CA	GLN	A	858	24.400	28.744	13.803	1.00	42.92
20	1554	C	GLN	A	858	22.927	28.400	13.731	1.00	43.62
	1555	O	GLN	A	858	22.173	29.017	12.988	1.00	47.41
	1556	CB	GLN	A	858	25.112	27.795	12.859	1.00	38.18
	1557	CG	GLN	A	858	26.563	28.061	12.645	1.00	41.30
25	1558	CD	GLN	A	858	27.216	26.990	11.788	1.00	48.05
	1559	OE1	GLN	A	858	28.399	27.051	11.521	1.00	60.25
	1560	NE2	GLN	A	858	26.446	25.995	11.369	1.00	53.15
30	1561	N	LEU	A	859	22.523	27.372	14.452	1.00	46.85
	1562	CA	LEU	A	859	21.136	26.956	14.407	1.00	44.50
	1563	C	LEU	A	859	20.226	27.884	15.180	1.00	41.57
	1564	O	LEU	A	859	19.091	28.129	14.764	1.00	41.55
35	1565	CB	LEU	A	859	20.998	25.529	14.919	1.00	49.03
	1566	CG	LEU	A	859	21.571	24.412	14.044	1.00	51.91
	1567	CD1	LEU	A	859	21.563	23.090	14.809	1.00	49.78
40	1568	CD2	LEU	A	859	20.736	24.301	12.793	1.00	54.19
	1569	N	THR	A	860	20.712	28.393	16.307	1.00	36.22
	1570	CA	THR	A	860	19.910	29.300	17.111	1.00	36.58
	1571	C	THR	A	860	19.694	30.592	16.322	1.00	39.98
45	1572	O	THR	A	860	18.600	31.177	16.351	1.00	41.71
	1573	CB	THR	A	860	20.557	29.532	18.474	1.00	35.81
	1574	OG1	THR	A	860	21.942	29.877	18.304	1.00	38.10
50	1575	CG2	THR	A	860	20.445	28.256	19.302	1.00	33.36
	1576	N	LYS	A	861	20.718	30.998	15.564	1.00	35.42
	1577	CA	LYS	A	861	20.598	32.178	14.715	1.00	38.56
	1578	C	LYS	A	861	19.556	31.871	13.639	1.00	44.29
55	1579	O	LYS	A	861	18.669	32.682	13.358	1.00	45.57
	1580	CB	LYS	A	861	21.932	32.530	14.076	1.00	35.42

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1581	CG	LYS	A	861	22.807	33.422	14.941	1.00	48.32
	1582	CD	LYS	A	861	22.394	34.906	14.850	1.00	56.04
	1583	CE	LYS	A	861	23.270	35.776	15.755	1.00	60.56
10	1584	NZ	LYS	A	861	22.863	37.205	15.751	1.00	65.17
	1585	N	LEU	A	862	19.644	30.667	13.075	1.00	46.55
	1586	CA	LEU	A	862	18.690	30.228	12.069	1.00	39.38
15	1587	C	LEU	A	862	17.272	30.273	12.642	1.00	40.85
	1588	O	LEU	A	862	16.353	30.720	11.954	1.00	45.44
	1589	CB	LEU	A	862	19.009	28.808	11.607	1.00	41.98
20	1590	CG	LEU	A	862	17.987	28.298	10.587	1.00	49.48
	1591	CD1	LEU	A	862	18.036	29.176	9.346	1.00	46.04
	1592	CD2	LEU	A	862	18.245	26.832	10.228	1.00	47.86
25	1593	N	LEU	A	863	17.108	29.839	13.900	1.00	38.85
	1594	CA	LEU	A	863	15.807	29.824	14.575	1.00	37.02
	1595	C	LEU	A	863	15.265	31.223	14.689	1.00	35.94
30	1596	O	LEU	A	863	14.075	31.459	14.455	1.00	36.06
	1597	CB	LEU	A	863	15.915	29.232	15.980	1.00	43.64
	1598	CG	LEU	A	863	15.888	27.707	16.086	1.00	42.37
35	1599	CD1	LEU	A	863	15.854	27.238	17.548	1.00	35.50
	1600	CD2	LEU	A	863	14.671	27.219	15.334	1.00	35.55
	1601	N	ASP	A	864	16.161	32.142	15.041	1.00	35.57
40	1602	CA	ASP	A	864	15.845	33.564	15.196	1.00	37.53
	1603	C	ASP	A	864	15.341	34.254	13.898	1.00	38.46
	1604	O	ASP	A	864	14.455	35.123	13.959	1.00	36.51
45	1605	CB	ASP	A	864	17.051	34.299	15.824	1.00	29.27
	1606	CG	ASP	A	864	17.214	34.005	17.334	1.00	39.10
	1607	OD1	ASP	A	864	16.388	33.270	17.927	1.00	42.54
50	1608	OD2	ASP	A	864	18.174	34.526	17.947	1.00	37.49
	1609	N	SER	A	865	15.843	33.796	12.740	1.00	40.46
	1610	CA	SER	A	865	15.476	34.302	11.393	1.00	35.87
55	1611	C	SER	A	865	14.004	34.116	11.058	1.00	37.22
	1612	O	SER	A	865	13.454	34.844	10.231	1.00	46.57
	1613	CB	SER	A	865	16.235	33.551	10.284	1.00	34.07
	1614	OG	SER	A	865	17.577	33.266	10.622	1.00	46.76
	1615	N	VAL	A	866	13.398	33.095	11.650	1.00	35.77
	1616	CA	VAL	A	866	12.013	32.752	11.399	1.00	35.13
	1617	C	VAL	A	866	11.031	33.779	11.950	1.00	38.58

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1618	O	VAL	A	866	9.973	34.057	11.353	1.00	36.20
1619	CB	VAL	A	866	11.686	31.354	12.004	1.00	27.91
1620	CG1	VAL	A	866	10.252	30.944	11.666	1.00	22.22
1621	CG2	VAL	A	866	12.666	30.322	11.482	1.00	33.78
1622	N	GLN	A	867	11.395	34.366	13.081	1.00	39.58
1623	CA	GLN	A	867	10.525	35.342	13.735	1.00	43.96
1624	C	GLN	A	867	10.213	36.633	12.921	1.00	38.67
1625	O	GLN	A	867	9.030	37.022	12.789	1.00	34.00
1626	CB	GLN	A	867	11.039	35.603	15.163	1.00	47.82
1627	CG	GLN	A	867	11.248	34.307	15.987	1.00	37.53
1628	CD	GLN	A	867	9.951	33.535	16.271	1.00	40.95
1629	OE1	GLN	A	867	8.841	33.972	15.943	1.00	40.47
1630	NE2	GLN	A	867	10.097	32.375	16.883	1.00	44.07
1631	N	PRO	A	868	11.254	37.306	12.370	1.00	32.90
1632	CA	PRO	A	868	11.071	38.522	11.569	1.00	32.84
1633	C	PRO	A	868	10.156	38.173	10.407	1.00	35.58
1634	O	PRO	A	868	9.132	38.815	10.173	1.00	34.36
1635	CB	PRO	A	868	12.477	38.796	11.052	1.00	34.85
1636	CG	PRO	A	868	13.329	38.358	12.184	1.00	35.76
1637	CD	PRO	A	868	12.690	37.069	12.631	1.00	35.45
1638	N	ILE	A	869	10.494	37.075	9.740	1.00	35.25
1639	CA	ILE	A	869	9.730	36.578	8.616	1.00	31.95
1640	C	ILE	A	869	8.284	36.304	9.002	1.00	28.05
1641	O	ILE	A	869	7.359	36.758	8.332	1.00	33.69
1642	CB	ILE	A	869	10.389	35.318	8.072	1.00	34.50
1643	CG1	ILE	A	869	11.841	35.639	7.697	1.00	31.97
1644	CG2	ILE	A	869	9.630	34.813	6.870	1.00	25.52
1645	CD1	ILE	A	869	12.604	34.477	7.120	1.00	36.91
1646	N	ALA	A	870	8.089	35.599	10.109	1.00	29.58
1647	CA	ALA	A	870	6.750	35.276	10.593	1.00	30.48
1648	C	ALA	A	870	6.010	36.567	10.913	1.00	34.81
1649	O	ALA	A	870	4.793	36.692	10.672	1.00	31.33
1650	CB	ALA	A	870	6.838	34.402	11.825	1.00	27.17
1651	N	ARG	A	871	6.754	37.534	11.441	1.00	35.08
1652	CA	ARG	A	871	6.201	38.845	11.766	1.00	38.73
1653	C	ARG	A	871	5.587	39.457	10.509	1.00	36.69
1654	O	ARG	A	871	4.411	39.824	10.496	1.00	33.58

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1655	CB	ARG	A	871	7.303	39.754	12.271	1.00	42.63
	1656	CG	ARG	A	871	6.935	41.209	12.267	1.00	48.87
	1657	CD	ARG	A	871	6.488	41.628	13.610	1.00	39.03
10	1658	NE	ARG	A	871	5.783	42.900	13.554	1.00	54.34
	1659	CZ	ARG	A	871	5.420	43.599	14.629	1.00	58.85
	1660	NH1	ARG	A	871	5.717	43.140	15.841	1.00	58.33
15	1661	NH2	ARG	A	871	4.700	44.713	14.497	1.00	67.98
	1662	N	GLU	A	872	6.388	39.518	9.447	1.00	33.87
	1663	CA	GLU	A	872	5.954	40.047	8.149	1.00	36.69
20	1664	C	GLU	A	872	4.721	39.346	7.610	1.00	35.07
	1665	O	GLU	A	872	3.835	39.982	7.039	1.00	38.97
	1666	CB	GLU	A	872	7.074	39.920	7.099	1.00	48.05
25	1667	CG	GLU	A	872	7.897	41.206	6.847	1.00	57.85
	1668	CD	GLU	A	872	8.928	41.037	5.731	1.00	68.10
	1669	OE1	GLU	A	872	9.952	40.366	5.990	1.00	74.25
30	1670	OE2	GLU	A	872	8.722	41.566	4.606	1.00	66.63
	1671	N	LEU	A	873	4.671	38.027	7.747	1.00	37.62
	1672	CA	LEU	A	873	3.528	37.281	7.244	1.00	35.57
35	1673	C	LEU	A	873	2.295	37.630	8.027	1.00	36.96
	1674	O	LEU	A	873	1.187	37.664	7.475	1.00	37.28
	1675	CB	LEU	A	873	3.794	35.790	7.331	1.00	46.12
40	1676	CG	LEU	A	873	5.003	35.377	6.498	1.00	44.82
	1677	CD1	LEU	A	873	5.185	33.921	6.706	1.00	46.86
	1678	CD2	LEU	A	873	4.807	35.680	5.024	1.00	41.83
45	1679	N	HIS	A	874	2.505	37.887	9.320	1.00	32.90
	1680	CA	HIS	A	874	1.430	38.269	10.242	1.00	37.34
	1681	C	HIS	A	874	0.775	39.603	9.828	1.00	38.25
50	1682	O	HIS	A	874	-0.457	39.758	9.814	1.00	36.81
	1683	CB	HIS	A	874	1.997	38.405	11.660	1.00	42.16
	1684	CG	HIS	A	874	2.251	37.099	12.352	1.00	46.12
55	1685	ND1	HIS	A	874	1.296	36.104	12.440	1.00	42.36
	1686	CD2	HIS	A	874	3.339	36.643	13.015	1.00	41.95
	1687	CE1	HIS	A	874	1.790	35.088	13.130	1.00	41.59
60	1688	NE2	HIS	A	874	3.028	35.390	13.486	1.00	44.61
	1689	N	GLN	A	875	1.628	40.572	9.520	1.00	38.39
	1690	CA	GLN	A	875	1.217	41.906	9.090	1.00	36.36
65	1691	C	GLN	A	875	0.363	41.731	7.845	1.00	34.57

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1692	O	GLN	A	875	-0.822	42.017	7.846	1.00	42.38
1693	CB	GLN	A	875	2.471	42.727	8.765	1.00	38.26
1694	CG	GLN	A	875	2.247	44.182	8.555	1.00	44.03
1695	CD	GLN	A	875	1.775	44.875	9.800	1.00	47.03
1696	OE1	GLN	A	875	2.554	45.079	10.754	1.00	42.92
1697	NE2	GLN	A	875	0.504	45.272	9.799	1.00	34.68
1698	N	PHE	A	876	0.943	41.081	6.849	1.00	33.26
1699	CA	PHE	A	876	0.284	40.845	5.582	1.00	33.07
1700	C	PHE	A	876	-1.070	40.161	5.677	1.00	35.06
1701	O	PHE	A	876	-2.036	40.573	5.032	1.00	34.48
1702	CB	PHE	A	876	1.212	40.017	4.692	1.00	39.86
1703	CG	PHE	A	876	0.676	39.782	3.313	1.00	39.61
1704	CD1	PHE	A	876	-0.320	38.846	3.085	1.00	41.67
1705	CD2	PHE	A	876	1.163	40.507	2.248	1.00	39.57
1706	CE1	PHE	A	876	-0.823	38.650	1.838	1.00	44.63
1707	CE2	PHE	A	876	0.665	40.318	0.991	1.00	40.20
1708	CZ	PHE	A	876	-0.329	39.385	0.780	1.00	49.53
1709	N	THR	A	877	-1.126	39.053	6.405	1.00	40.28
1710	CA	THR	A	877	-2.380	38.320	6.505	1.00	38.84
1711	C	THR	A	877	-3.450	39.157	7.208	1.00	41.69
1712	O	THR	A	877	-4.594	39.193	6.767	1.00	41.63
1713	CB	THR	A	877	-2.193	36.900	7.135	1.00	33.79
1714	OG1	THR	A	877	-3.364	36.117	6.886	1.00	38.07
1715	CG2	THR	A	877	-1.937	36.956	8.640	1.00	26.06
1716	N	PHE	A	878	-3.062	39.889	8.251	1.00	39.96
1717	CA	PHE	A	878	-3.997	40.737	8.984	1.00	38.02
1718	C	PHE	A	878	-4.600	41.760	8.006	1.00	38.85
1719	O	PHE	A	878	-5.821	41.922	7.916	1.00	33.84
1720	CB	PHE	A	878	-3.248	41.450	10.109	1.00	41.25
1721	CG	PHE	A	878	-4.035	42.540	10.764	1.00	45.72
1722	CD1	PHE	A	878	-5.318	42.298	11.237	1.00	47.19
1723	CD2	PHE	A	878	-3.490	43.810	10.910	1.00	47.82
1724	CE1	PHE	A	878	-6.045	43.296	11.842	1.00	52.43
1725	CE2	PHE	A	878	-4.208	44.813	11.515	1.00	44.62
1726	CZ	PHE	A	878	-5.488	44.563	11.983	1.00	50.04
1727	N	ASP	A	879	-3.717	42.398	7.243	1.00	41.64
1728	CA	ASP	A	879	-4.078	43.395	6.242	1.00	44.39

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1729	C	ASP	A	879	-4.975	42.733	5.201	41.74
	1730	O	ASP	A	879	-6.013	43.272	4.797	45.58
	1731	CB	ASP	A	879	-2.799	43.987	5.597	50.23
10	1732	CG	ASP	A	879	-1.938	44.849	6.595	65.18
	1733	OD1	ASP	A	879	-2.253	44.919	7.821	64.91
	1734	OD2	ASP	A	879	-0.930	45.461	6.140	57.87
	1735	N	LEU	A	880	-4.581	41.542	4.784	39.59
15	1736	CA	LEU	A	880	-5.349	40.778	3.824	41.16
	1737	C	LEU	A	880	-6.737	40.477	4.404	41.39
	1738	O	LEU	A	880	-7.720	40.472	3.682	46.61
20	1739	CB	LEU	A	880	-4.594	39.483	3.484	41.26
	1740	CG	LEU	A	880	-5.117	38.492	2.429	46.22
	1741	CD1	LEU	A	880	-5.910	39.174	1.299	39.53
	1742	CD2	LEU	A	880	-3.925	37.702	1.873	45.58
25	1743	N	LEU	A	881	-6.826	40.273	5.713	46.94
	1744	CA	LEU	A	881	-8.113	39.974	6.330	46.60
	1745	C	LEU	A	881	-9.028	41.185	6.310	50.61
30	1746	O	LEU	A	881	-10.188	41.070	5.925	50.82
	1747	CB	LEU	A	881	-7.964	39.468	7.775	38.43
	1748	CG	LEU	A	881	-9.282	39.274	8.551	37.70
	1749	CD1	LEU	A	881	-10.162	38.204	7.887	30.98
35	1750	CD2	LEU	A	881	-8.979	38.918	9.997	30.24
	1751	N	ILE	A	882	-8.531	42.341	6.746	48.70
	1752	CA	ILE	A	882	-9.390	43.517	6.752	55.61
40	1753	C	ILE	A	882	-9.806	43.885	5.314	53.19
	1754	O	ILE	A	882	-10.966	44.227	5.076	56.55
	1755	CB	ILE	A	882	-8.797	44.720	7.603	54.73
45	1756	CG1	ILE	A	882	-7.489	45.252	7.008	58.00
	1757	CG2	ILE	A	882	-8.566	44.271	9.054	42.17
	1758	CD1	ILE	A	882	-6.825	46.382	7.811	61.98
	1759	N	LYS	A	883	-8.917	43.674	4.343	51.98
50	1760	CA	LYS	A	883	-9.229	43.976	2.939	53.80
	1761	C	LYS	A	883	-10.126	42.935	2.296	56.69
	1762	O	LYS	A	883	-10.888	43.257	1.389	56.03
55	1763	CB	LYS	A	883	-7.976	44.008	2.073	49.48
	1764	CG	LYS	A	883	-7.056	45.152	2.279	51.98
	1765	CD	LYS	A	883	-5.970	45.061	1.236	57.39

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1766	CE	LYS	A	883	-4.752	45.885	1.601	1.00	65.28
1767	NZ	LYS	A	883	-3.755	45.773	0.507	1.00	72.32
1768	N	SER	A	884	-10.000	41.687	2.758	1.00	64.45
1769	CA	SER	A	884	-10.721	40.515	2.228	1.00	60.51
1770	C	SER	A	884	-12.055	40.765	1.543	1.00	57.37
1771	O	SER	A	884	-12.167	40.549	0.334	1.00	55.96
1772	CB	SER	A	884	-10.873	39.434	3.304	1.00	60.86
1773	OG	SER	A	884	-11.559	39.933	4.437	1.00	69.00
1774	N	HIS	A	885	-13.029	41.258	2.308	1.00	59.05
1775	CA	HIS	A	885	-14.376	41.558	1.826	1.00	68.14
1776	C	HIS	A	885	-14.388	42.167	0.424	1.00	74.11
1777	O	HIS	A	885	-14.901	41.561	-0.515	1.00	78.87
1778	CB	HIS	A	885	-15.091	42.532	2.781	1.00	74.25
1779	CG	HIS	A	885	-14.848	42.258	4.241	1.00	79.02
1780	ND1	HIS	A	885	-13.766	42.770	4.919	1.00	75.36
1781	CD2	HIS	A	885	-15.545	41.521	5.135	1.00	74.74
1782	CE1	HIS	A	885	-13.802	42.360	6.178	1.00	69.84
1783	NE2	HIS	A	885	-14.871	41.599	6.335	1.00	76.42
1784	N	MET	A	886	-13.813	43.358	0.284	1.00	77.20
1785	CA	MET	A	886	-13.780	44.065	-1.003	1.00	75.99
1786	C	MET	A	886	-12.804	43.540	-2.083	1.00	66.55
1787	O	MET	A	886	-12.844	44.000	-3.225	1.00	63.97
1788	CB	MET	A	886	-13.570	45.582	-0.755	1.00	87.39
1789	CG	MET	A	886	-12.135	46.127	-0.979	1.00	94.48
1790	SD	MET	A	886	-11.788	47.728	-0.157	1.00	94.87
1791	CE	MET	A	886	-10.212	48.246	-1.001	1.00	94.14
1792	N	VAL	A	887	-11.942	42.584	-1.738	1.00	60.32
1793	CA	VAL	A	887	-10.968	42.057	-2.702	1.00	54.75
1794	C	VAL	A	887	-11.146	40.564	-3.026	1.00	56.80
1795	O	VAL	A	887	-10.263	39.931	-3.624	1.00	52.84
1796	CB	VAL	A	887	-9.525	42.334	-2.213	1.00	48.73
1797	CG1	VAL	A	887	-9.081	41.277	-1.221	1.00	55.82
1798	CG2	VAL	A	887	-8.578	42.459	-3.377	1.00	42.79
1799	N	SER	A	888	-12.293	40.033	-2.599	1.00	60.63
1800	CA	SER	A	888	-12.752	38.643	-2.786	1.00	60.83
1801	C	SER	A	888	-11.912	37.401	-2.406	1.00	65.27
1802	O	SER	A	888	-12.196	36.292	-2.885	1.00	62.05

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1803	CB	SER	A	888	-13.368	38.463	-4.169	1.00	51.52
	1804	OG	SER	A	888	-12.417	38.680	-5.181	1.00	58.27
	1805	N	VAL	A	889	-10.918	37.579	-1.529	1.00	70.51
10	1806	CA	VAL	A	889	-10.079	36.475	-1.036	1.00	69.77
	1807	C	VAL	A	889	-10.894	35.856	0.115	1.00	71.90
	1808	O	VAL	A	889	-11.475	36.609	0.910	1.00	70.16
15	1809	CB	VAL	A	889	-8.740	37.003	-0.461	1.00	68.58
	1810	CG1	VAL	A	889	-7.880	35.843	-0.016	1.00	73.27
	1811	CG2	VAL	A	889	-8.006	37.859	-1.489	1.00	65.97
20	1812	N	ASP	A	890	-10.969	34.520	0.203	1.00	74.76
	1813	CA	ASP	A	890	-11.758	33.870	1.271	1.00	72.71
	1814	C	ASP	A	890	-10.920	33.314	2.457	1.00	69.55
25	1815	O	ASP	A	890	-9.783	32.831	2.270	1.00	70.86
	1816	CB	ASP	A	890	-12.783	32.857	0.666	1.00	72.91
	1817	CG	ASP	A	890	-12.332	31.385	0.735	1.00	80.84
30	1818	OD1	ASP	A	890	-11.326	30.981	0.093	1.00	76.21
	1819	OD2	ASP	A	890	-13.045	30.618	1.413	1.00	78.59
	1820	N	PHE	A	891	-11.431	33.508	3.680	1.00	59.70
35	1821	CA	PHE	A	891	-10.746	33.068	4.902	1.00	52.91
	1822	C	PHE	A	891	-11.598	32.045	5.665	1.00	49.30
	1823	O	PHE	A	891	-12.740	32.326	6.012	1.00	50.65
40	1824	CB	PHE	A	891	-10.474	34.274	5.848	1.00	55.80
	1825	CG	PHE	A	891	-9.223	35.088	5.518	1.00	47.41
	1826	CD1	PHE	A	891	-9.250	36.101	4.554	1.00	40.14
45	1827	CD2	PHE	A	891	-8.027	34.837	6.171	1.00	45.78
	1828	CE1	PHE	A	891	-8.107	36.842	4.246	1.00	34.67
	1829	CE2	PHE	A	891	-6.876	35.585	5.862	1.00	46.05
50	1830	CZ	PHE	A	891	-6.922	36.582	4.900	1.00	37.02
	1831	N	PRO	A	892	-11.052	30.845	5.926	1.00	44.99
	1832	CA	PRO	A	892	-11.782	29.806	6.660	1.00	39.76
55	1833	C	PRO	A	892	-11.976	30.370	8.058	1.00	44.96
	1834	O	PRO	A	892	-11.052	30.952	8.621	1.00	46.87
	1835	CB	PRO	A	892	-10.792	28.648	6.669	1.00	45.27
55	1836	CG	PRO	A	892	-9.970	28.878	5.420	1.00	46.05
	1837	CD	PRO	A	892	-9.737	30.353	5.480	1.00	46.20
	1838	N	GLU	A	893	-13.176	30.234	8.604	1.00	51.64
	1839	CA	GLU	A	893	-13.508	30.792	9.914	1.00	51.25

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1840	C	GLU	A	893	-12.577	30.549	11.077	1.00	52.74
1841	O	GLU	A	893	-12.321	31.462	11.858	1.00	58.39
1842	CB	GLU	A	893	-14.937	30.437	10.304	1.00	59.05
1843	CG	GLU	A	893	-15.987	31.401	9.724	1.00	75.65
1844	CD	GLU	A	893	-15.800	31.699	8.224	1.00	82.95
1845	OE1	GLU	A	893	-15.706	30.745	7.418	1.00	84.06
1846	OE2	GLU	A	893	-15.762	32.891	7.845	1.00	86.37
1847	N	MET	A	894	-12.043	29.348	11.205	1.00	52.94
1848	CA	MET	A	894	-11.152	29.075	12.329	1.00	57.23
1849	C	MET	A	894	-9.942	29.975	12.239	1.00	57.71
1850	O	MET	A	894	-9.458	30.518	13.230	1.00	60.99
1851	CB	MET	A	894	-10.720	27.607	12.332	1.00	59.88
1852	CG	MET	A	894	-9.861	27.205	13.522	1.00	68.32
1853	SD	MET	A	894	-9.861	25.428	13.821	1.00	73.67
1854	CE	MET	A	894	-9.322	24.840	12.166	1.00	72.54
1855	N	MET	A	895	-9.466	30.130	11.021	1.00	61.08
1856	CA	MET	A	895	-8.311	30.948	10.744	1.00	58.05
1857	C	MET	A	895	-8.679	32.431	10.789	1.00	56.79
1858	O	MET	A	895	-7.979	33.226	11.422	1.00	56.34
1859	CB	MET	A	895	-7.751	30.527	9.396	1.00	57.93
1860	CG	MET	A	895	-6.936	31.548	8.720	1.00	67.27
1861	SD	MET	A	895	-6.668	30.991	7.072	1.00	79.81
1862	CE	MET	A	895	-4.870	31.161	6.982	1.00	78.99
1863	N	ALA	A	896	-9.786	32.802	10.152	1.00	49.66
1864	CA	ALA	A	896	-10.219	34.186	10.170	1.00	46.91
1865	C	ALA	A	896	-10.211	34.621	11.627	1.00	50.19
1866	O	ALA	A	896	-9.655	35.672	11.971	1.00	55.53
1867	CB	ALA	A	896	-11.616	34.311	9.591	1.00	45.04
1868	N	GLU	A	897	-10.737	33.759	12.496	1.00	52.29
1869	CA	GLU	A	897	-10.805	34.053	13.928	1.00	52.77
1870	C	GLU	A	897	-9.442	34.244	14.591	1.00	48.32
1871	O	GLU	A	897	-9.253	35.144	15.402	1.00	49.52
1872	CB	GLU	A	897	-11.612	32.990	14.664	1.00	54.94
1873	CG	GLU	A	897	-11.927	33.355	16.111	1.00	65.44
1874	CD	GLU	A	897	-13.217	32.725	16.600	1.00	75.27
1875	OE1	GLU	A	897	-14.284	33.102	16.074	1.00	78.93
1876	OE2	GLU	A	897	-13.167	31.868	17.511 1	1.00	79.28

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1877	N	ILE	A	898	-8.477	33.417	14.241	1.00	45.91
	1878	CA	ILE	A	898	-7.160	33.561	14.836	1.00	43.63
	1879	C	ILE	A	898	-6.510	34.843	14.323	1.00	41.42
10	1880	O	ILE	A	898	-5.891	35.578	15.087	1.00	41.91
	1881	CB	ILE	A	898	-6.275	32.288	14.567	1.00	45.82
	1882	CG1	ILE	A	898	-6.797	31.125	15.430	1.00	48.14
15	1883	CG2	ILE	A	898	-4.776	32.537	14.847	1.00	34.18
	1884	CD1	ILE	A	898	-5.911	29.894	15.425	1.00	60.11
	1885	N	ILE	A	899	-6.734	35.177	13.064	1.00	37.89
20	1886	CA	ILE	A	899	-6.105	36.372	12.526	1.00	40.46
	1887	C	ILE	A	899	-6.640	37.624	13.202	1.00	39.91
	1888	O	ILE	A	899	-5.880	38.533	13.524	1.00	36.62
25	1889	CB	ILE	A	899	-6.290	36.486	10.986	1.00	46.34
	1890	CG1	ILE	A	899	-5.722	35.250	10.280	1.00	51.08
	1891	CG2	ILE	A	899	-5.612	37.759	10.448	1.00	45.77
30	1892	CD1	ILE	A	899	-4.239	34.978	10.550	1.00	53.92
	1893	N	SER	A	900	-7.927	37.612	13.520	1.00	39.54
	1894	CA	SER	A	900	-8.576	38.764	14.129	1.00	39.63
35	1895	C	SER	A	900	-8.474	38.925	15.652	1.00	41.36
	1896	O	SER	A	900	-8.821	39.970	16.188	1.00	46.90
	1897	CB	SER	A	900	-10.048	38.823	13.670	1.00	37.01
40	1898	OG	SER	A	900	-10.963	38.377	14.652	1.00	40.29
	1899	N	VAL	A	901	-7.942	37.938	16.350	1.00	34.58
	1900	CA	VAL	A	901	-7.889	38.027	17.799	1.00	32.25
45	1901	C	VAL	A	901	-6.516	37.812	18.388	1.00	33.93
	1902	O	VAL	A	901	-6.116	38.496	19.325	1.00	37.49
	1903	CB	VAL	A	901	-8.844	36.967	18.443	1.00	40.69
50	1904	CG1	VAL	A	901	-8.793	37.045	19.976	1.00	37.09
	1905	CG2	VAL	A	901	-10.273	37.146	17.930	1.00	37.39
	1906	N	GLN	A	902	-5.813	36.820	17.865	1.00	38.32
55	1907	CA	GLN	A	902	-4.504	36.475	18.376	1.00	36.30
	1908	C	GLN	A	902	-3.432	37.222	17.639	1.00	39.26
	1909	O	GLN	A	902	-2.419	37.566	18.234	1.00	41.22
60	1910	CB	GLN	A	902	-4.247	34.958	18.276	1.00	36.78
	1911	CG	GLN	A	902	-5.309	34.053	18.926	1.00	41.09
	1912	CD	GLN	A	902	-5.529	34.320	20.418	1.00	47.88
65	1913	OE1	GLN	A	902	-6.664	34.277	20.899	1.00	56.15

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1914	NE2	GLN	A	902	-4.447	34.587	21.155	1.00	43.52
	1915	N	VAL	A	903	-3.621	37.449	16.340	1.00	40.86
	1916	CA	VAL	A	903	-2.611	38.167	15.569	1.00	38.57
	1917	C	VAL	A	903	-2.431	39.624	16.026	1.00	37.36
10	1918	O	VAL	A	903	-1.294	40.077	16.171	1.00	39.48
	1919	CB	VAL	A	903	-2.841	38.035	14.028	1.00	42.29
	1920	CG1	VAL	A	903	-1.947	38.994	13.270	1.00	39.28
15	1921	CG2	VAL	A	903	-2.503	36.622	13.574	1.00	39.72
	1922	N	PRO	A	904	-3.534	40.366	16.292	1.00	30.75
	1923	CA	PRO	A	904	-3.373	41.753	16.738	1.00	32.91
	1924	C	PRO	A	904	-2.436	41.878	17.945	1.00	36.72
20	1925	O	PRO	A	904	-1.624	42.801	18.019	1.00	40.29
	1926	CB	PRO	A	904	-4.797	42.161	17.092	1.00	29.43
	1927	CG	PRO	A	904	-5.571	41.493	16.035	1.00	30.40
25	1928	CD	PRO	A	904	-4.962	40.088	16.042	1.00	34.37
	1929	N	LYS	A	905	-2.489	40.909	18.851	1.00	36.01
	1930	CA	LYS	A	905	-1.632	40.937	20.031	1.00	32.07
30	1931	C	LYS	A	905	-0.149	40.868	19.677	1.00	30.44
	1932	O	LYS	A	905	0.688	41.365	20.422	1.00	33.55
	1933	CB	LYS	A	905	-1.995	39.807	21.022	1.00	34.01
	1934	CG	LYS	A	905	-3.485	39.698	21.377	1.00	37.81
35	1935	CD	LYS	A	905	-3.751	38.653	22.476	1.00	51.29
	1936	CE	LYS	A	905	-5.233	38.624	22.886	1.00	51.15
	1937	NZ	LYS	A	905	-5.552	37.658	23.987	1.00	63.78
40	1938	N	ILE	A	906	0.185	40.258	18.545	1.00	38.99
	1939	CA	ILE	A	906	1.588	40.103	18.142	1.00	43.43
	1940	C	ILE	A	906	2.076	41.353	17.449	1.00	46.59
	1941	O	ILE	A	906	3.203	41.817	17.688	1.00	46.25
45	1942	CB	ILE	A	906	1.818	38.828	17.217	1.00	41.03
	1943	CG1	ILE	A	906	1.453	37.545	17.993	1.00	41.68
	1944	CG2	ILE	A	906	3.289	38.764	16.745	1.00	35.00
50	1945	CD1	ILE	A	906	1.386	36.270	17.189	1.00	36.91
	1946	N	LEU	A	907	1.217	41.891	16.587	1.00	50.54
	1947	CA	LEU	A	907	1.516	43.111	15.831	1.00	47.53
	1948	C	LEU	A	907	1.639	44.317	16.784	1.00	42.06
55	1949	O	LEU	A	907	2.496	45.199	16.590	1.00	41.92
	1950	CB	LEU	A	907	0.437	43.324	14.751	1.00	43.43

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1951	CG	LEU	A	907	0.323	42.131	13.782	1.00	31.27
	1952	CD1	LEU	A	907	-0.857	42.290	12.901	1.00	29.15
	1953	CD2	LEU	A	907	1.580	41.967	12.953	1.00	29.66
10	1954	N	SER	A	908	0.851	44.282	17.858	1.00	36.02
	1955	CA	SER	A	908	0.871	45.328	18.852	1.00	41.77
	1956	C	SER	A	908	1.943	45.131	19.931	1.00	45.83
	1957	O	SER	A	908	2.115	45.985	20.788	1.00	57.61
15	1958	CB	SER	A	908	-0.519	45.531	19.479	1.00	44.15
	1959	OG	SER	A	908	-0.913	44.474	20.334	1.00	47.22
	1960	N	GLY	A	909	2.684	44.030	19.886	1.00	40.63
20	1961	CA	GLY	A	909	3.726	43.813	20.877	1.00	31.68
	1962	C	GLY	A	909	3.324	43.227	22.233	1.00	37.71
	1963	O	GLY	A	909	4.173	43.163	23.129	1.00	42.65
	1964	N	LYS	A	910	2.071	42.791	22.401	1.00	33.50
25	1965	CA	LYS	A	910	1.619	42.182	23.673	1.00	42.03
	1966	C	LYS	A	910	2.064	40.702	23.839	1.00	41.10
	1967	O	LYS	A	910	2.036	40.137	24.932	1.00	39.99
	1968	CB	LYS	A	910	0.100	42.320	23.805	1.00	41.10
30	1969	CG	LYS	A	910	-0.357	43.751	23.582	1.00	45.52
	1970	CD	LYS	A	910	-1.830	43.904	23.726	1.00	40.97
	1971	CE	LYS	A	910	-2.190	43.976	25.163	1.00	42.32
	1972	NZ	LYS	A	910	-3.651	43.819	25.260	1.00	53.43
35	1973	N	VAL	A	911	2.497	40.114	22.728	1.00	42.05
	1974	CA	VAL	A	911	2.992	38.746	22.624	1.00	35.21
	1975	C	VAL	A	911	4.267	38.912	21.806	1.00	36.16
	1976	O	VAL	A	911	4.224	39.387	20.671	1.00	37.87
40	1977	CB	VAL	A	911	2.025	37.872	21.822	1.00	29.65
	1978	CG1	VAL	A	911	2.661	36.551	21.476	1.00	33.30
	1979	CG2	VAL	A	911	0.736	37.674	22.588	1.00	35.10
	1980	N	LYS	A	912	5.396	38.504	22.358	1.00	35.80
45	1981	CA	LYS	A	912	6.638	38.677	21.653	1.00	36.47
	1982	C	LYS	A	912	7.451	37.409	21.556	1.00	40.23
	1983	O	LYS	A	912	7.293	36.472	22.334	1.00	39.68
	1984	CB	LYS	A	912	7.483	39.752	22.347	1.00	37.13
50	1985	CG	LYS	A	912	7.952	39.353	23.729	0.00	38.33
	1986	CD	LYS	A	912	8.846	40.405	24.332	0.00	39.07
	1987	CE	LYS	A	912	9.124	40.089	25.784	0.00	39.77

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1988	NZ	LYS	A	912	9.862	41.200	26.423	0.00	40.28
1989	N	PRO	A	913	8.266	37.333	20.517	1.00	39.61
1990	CA	PRO	A	913	9.146	36.208	20.249	1.00	40.14
1991	C	PRO	A	913	10.247	36.181	21.301	1.00	36.50
1992	O	PRO	A	913	10.565	37.200	21.893	1.00	38.67
1993	CB	PRO	A	913	9.711	36.564	18.875	1.00	41.93
1994	CG	PRO	A	913	8.534	37.200	18.210	1.00	44.72
1995	CD	PRO	A	913	8.060	38.134	19.296	1.00	42.22
1996	N	ILE	A	914	10.813	35.008	21.538	1.00	34.68
1997	CA	ILE	A	914	11.883	34.848	22.497	1.00	36.82
1998	C	ILE	A	914	13.085	34.508	21.654	1.00	40.11
1999	O	ILE	A	914	13.129	33.460	21.029	1.00	43.44
2000	CB	ILE	A	914	11.625	33.663	23.434	1.00	38.93
2001	CG1	ILE	A	914	10.311	33.834	24.173	1.00	32.49
2002	CG2	ILE	A	914	12.743	33.540	24.435	1.00	46.36
2003	CD1	ILE	A	914	9.917	32.567	24.899	1.00	39.70
2004	N	TYR	A	915	14.047	35.409	21.603	1.00	45.62
2005	CA	TYR	A	915	15.235	35.191	20.798	1.00	45.53
2006	C	TYR	A	915	16.352	34.582	21.608	1.00	47.03
2007	O	TYR	A	915	16.359	34.665	22.833	1.00	51.25
2008	CB	TYR	A	915	15.717	36.510	20.165	1.00	38.58
2009	CG	TYR	A	915	14.778	37.052	19.122	1.00	36.78
2010	CD1	TYR	A	915	13.600	37.695	19.484	1.00	38.75
2011	CD2	TYR	A	915	15.042	36.875	17.767	1.00	47.40
2012	CE1	TYR	A	915	12.696	38.141	18.527	1.00	49.22
2013	CE2	TYR	A	915	14.142	37.317	16.786	1.00	52.13
2014	CZ	TYR	A	915	12.969	37.952	17.175	1.00	56.55
2015	OH	TYR	A	915	12.067	38.377	16.212	1.00	55.66
2016	N	PHE	A	916	17.298	33.964	20.915	1.00	46.26
2017	CA	PHE	A	916	18.439	33.376	21.580	1.00	44.65
2018	C	PHE	A	916	19.487	34.457	21.707	1.00	44.05
2019	O	PHE	A	916	20.132	34.568	22.738	1.00	47.61
2020	CB	PHE	A	916	18.993	32.180	20.787	1.00	42.46
2021	CG	PHE	A	916	18.213	30.915	20.991	1.00	44.06
2022	CD1	PHE	A	916	17.006	30.705	20.326	1.00	46.38
2023	CD2	PHE	A	916	18.670	29.948	21.875	1.00	47.18
2024	CE1	PHE	A	916	16.263	29.553	20.540	1.00	45.51

TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2025	CE2	PHE	A	916	17.939	28.789	22.098	1.00	46.95
	2026	CZ	PHE	A	916	16.732	28.594	21.426	1.00	45.10
	2027	N	HIS	A	917	19.603	35.303	20.689	1.00	46.97
10	2028	CA	HIS	A	917	20.611	36.352	20.694	1.00	47.06
	2029	C	HIS	A	917	20.043	37.777	20.743	1.00	52.16
	2030	O	HIS	A	917	20.353	38.603	19.896	1.00	57.53
15	2031	CB	HIS	A	917	21.524	36.170	19.471	1.00	49.03
	2032	CG	HIS	A	917	21.994	34.756	19.246	1.00	43.80
	2033	ND1	HIS	A	917	23.287	34.340	19.494	1.00	47.63
20	2034	CD2	HIS	A	917	21.343	33.670	18.762	1.00	48.20
	2035	CE1	HIS	A	917	23.414	33.065	19.173	1.00	51.22
	2036	NE2	HIS	A	917	22.248	32.631	18.726	1.00	47.78
25	2037	N	THR	A	918	19.206	38.052	21.735	1.00	62.03
	2038	CA	THR	A	918	18.597	39.381	21.917	1.00	72.18
	2039	C	THR	A	918	19.558	40.395	22.571	1.00	75.33
30	2040	O	THR	A	918	19.150	41.565	22.781	1.00	78.71
	2041	CB	THR	A	918	17.378	39.309	22.847	1.00	73.07
	2042	OG1	THR	A	918	16.840	37.980	22.842	1.00	72.53
35	2043	CG2	THR	A	918	16.301	40.339	22.419	1.00	76.16
	2044	OXT	THR	A	918	20.674	39.997	22.964	1.00	76.97
	2045		THR	A	918					
40	2046	C1	R18	A	1000	0.414	28.070	4.103	1.00	47.66
	2047	C2	R18	A	1000	1.195	26.999	4.832	1.00	49.34
	2048	C3	R18	A	1000	2.661	27.140	4.532	1.00	53.90
45	2049	C4	R18	A	1000	3.174	28.457	4.794	1.00	55.05
	2050	C5	R18	A	1000	2.367	29.553	4.780	1.00	50.29
	2051	C6	R18	A	1000	2.973	30.906	5.116	1.00	47.48
50	2052	C7	R18	A	1000	2.207	32.030	4.457	1.00	46.11
	2053	C8	R18	A	1000	0.733	31.962	4.898	1.00	45.61
	2054	C9	R18	A	1000	0.124	30.597	4.514	1.00	49.94
55	2055	C10	R18	A	1000	0.912	29.480	4.476	1.00	49.84
	2056	C11	R18	A	1000	-1.316	30.583	4.251	1.00	47.61
	2057	C12	R18	A	1000	-2.102	31.675	4.310	1.00	47.26
60	2058	C13	R18	A	1000	-1.535	33.039	4.664	1.00	44.26
	2059	C14	R18	A	1000	-0.056	33.066	4.261	1.00	42.93
	2060	C15	R18	A	1000	0.387	34.509	4.572	1.00	43.22
65	2061	C16	R18	A	1000	-0.899	35.299	4.311	1.00	41.50

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TABLE 9 (continued)

THREE-DIMENSIONAL COORDINATES OF AR IN COMPLEX WITH THE LIGAND R1881									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2062	C17	R18	A	1000	-2.001	34.282	3.900	1.00	43.39
2063	C18	R18	A	1000	-1.725	33.228	6.189	1.00	41.74
2064	C27	R18	A	1000	-2.034	34.050	2.412	1.00	40.38
2065	O83	R18	A	1000	3.375	26.212	4.162	1.00	59.41
2066	O97	R18	A	1000	-3.257	34.797	4.345	1.00	48.46
2067	O	HOH	Z	1	17.517	11.963	20.575	1.00	51.58
2068	O	HOH	Z	2	7.977	16.353	14.548	1.00	29.86
2069	O	HOH	Z	3	3.112	18.553	3.147	1.00	65.78
2070	O	HOH	Z	4	1.314	20.835	2.312	1.00	46.40
2071	O	HOH	Z	5	0.422	24.646	-12.882	1.00	58.80
2072	O	HOH	Z	6	-1.370	30.527	-15.016	1.00	41.87
2073	O	HOH	Z	7	-4.737	36.972	-13.426	1.00	75.71
2074	O	HOH	Z	8	4.151	24.024	6.333	1.00	32.89
2075	O	HOH	Z	9	-7.536	14.518	23.118	1.00	42.77
2076	O	HOH	Z	10	1.368	26.376	31.674	1.00	49.63
2077	O	HOH	Z	11	1.207	32.439	14.426	1.00	45.58
2078	O	HOH	Z	12	4.179	32.582	14.418	1.00	31.77
2079	O	HOH	Z	13	-5.348	34.883	24.137	1.00	62.76
2080	O	HOH	Z	14	2.739	25.007	-10.984	1.00	53.83
2081	O	HOH	Z	15	10.790	29.074	3.632	1.00	61.00
2082	O	HOH	Z	16	18.090	34.834	6.262	1.00	66.21
2083	O	HOH	Z	17	28.211	24.615	5.938	1.00	56.69
2084	O	HOH	Z	18	5.741	29.774	22.458	1.00	37.52
2085	O	HOH	Z	19	12.529	31.030	16.979	1.00	35.29
2086	O	HOH	Z	20	7.674	37.499	32.487	1.00	46.92
2087	O	HOH	Z	21	26.453	8.689	17.052	1.00	48.49
2088	O	HOH	Z	22	7.032	36.581	14.890	1.00	40.54
2089	O	HOH	Z	23	6.659	32.126	15.319	1.00	44.19
2090	O	HOH	Z	24	2.693	46.635	13.278	1.00	46.55
2091	O	HOH	Z	25	5.869	40.798	18.893	1.00	48.79
2092	O	HOH	Z	26	16.821	36.244	25.158	1.00	58.36

TABLE 10

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1	N	GLN	A	682	31.180	-1.959	93.866	1.00	69.36
2	CA	GLN	A	682	32.157	-2.958	94.388	1.00	66.54

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3	C	GLN	A	682	33.310	-3.159	93.410	1.00	66.47
	4	O	GLN	A	682	34.414	-2.653	93.627	1.00	66.82
	5	CB	GLN	A	682	31.453	-4.285	94.646	1.00	68.47
10	6	N	LEU	A	683	33.053	-3.900	92.336	1.00	63.30
	7	CA	LEU	A	683	34.077	-4.153	91.334	1.00	60.85
	8	C	LEU	A	683	34.028	-3.134	90.197	1.00	56.94
15	9	O	LEU	A	683	35.057	-2.832	89.590	1.00	54.60
	10	CB	LEU	A	683	33.941	-5.573	90.767	1.00	61.13
	11	CG	LEU	A	683	34.171	-6.734	91.743	1.00	66.50
20	12	CD1	LEU	A	683	34.044	-8.065	91.003	1.00	60.00
	13	CD2	LEU	A	683	35.555	-6.617	92.370	1.00	59.53
	14	N	ILE	A	684	32.839	-2.607	89.911	1.00	52.97
25	15	CA	ILE	A	684	32.696	-1.624	88.844	1.00	48.69
	16	C	ILE	A	684	33.249	-0.282	89.320	1.00	46.25
	17	O	ILE	A	684	32.771	0.276	90.302	1.00	41.04
30	18	CB	ILE	A	684	31.219	-1.426	88.437	1.00	52.18
	19	CG1	ILE	A	684	30.594	-2.764	88.029	1.00	50.50
	20	CG2	ILE	A	684	31.137	-0.448	87.269	1.00	48.24
35	21	CD1	ILE	A	684	31.258	-3.423	86.839	1.00	51.57
	22	N	PRO	A	685	34.270	0.250	88.628	1.00	40.66
	23	CA	PRO	A	685	34.874	1.532	89.001	1.00	39.82
40	24	C	PRO	A	685	33.846	2.665	89.084	1.00	36.13
	25	O	PRO	A	685	32.885	2.697	88.319	1.00	35.64
	26	CB	PRO	A	685	35.913	1.743	87.901	1.00	34.22
45	27	CG	PRO	A	685	36.328	0.330	87.591	1.00	43.36
	28	CD	PRO	A	685	34.951	-0.290	87.441	1.00	40.38
	29	N	PRO	A	686	34.049	3.610	90.013	1.00	35.29
50	30	CA	PRO	A	686	33.161	4.756	90.234	1.00	35.12
	31	C	PRO	A	686	32.856	5.569	88.978	1.00	30.01
	32	O	PRO	A	686	31.698	5.883	88.696	1.00	29.64
55	33	CB	PRO	A	686	33.923	5.573	91.275	1.00	36.34
	34	CG	PRO	A	686	34.626	4.484	92.076	1.00	41.25
	35	CD	PRO	A	686	35.210	3.700	90.919	1.00	39.57
55	36	N	LEU	A	687	33.901	5.907	88.231	1.00	29.04
	37	CA	LEU	A	687	33.729	6.701	87.013	1.00	28.23
	38	C	LEU	A	687	32.874	5.982	85.970	1.00	26.62
	39	O	LEU	A	687	32.096	6.607	85.240	1.00	25.82

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	40	CB	LEU	A	687	35.086	7.048	86.422	1.00	25.68
	41	CG	LEU	A	687	35.023	7.915	85.165	1.00	34.63
	42	CD1	LEU	A	687	34.104	9.118	85.408	1.00	30.55
10	43	CD2	LEU	A	687	36.436	8.348	84.790	1.00	30.65
	44	N	ILE	A	688	33.015	4.663	85.898	1.00	27.06
	45	CA	ILE	A	688	32.226	3.891	84.951	1.00	23.18
15	46	C	ILE	A	688	30.762	3.860	85.377	1.00	24.05
	47	O	ILE	A	688	29.859	3.990	84.545	1.00	26.77
	48	CB	ILE	A	688	32.788	2.477	84.815	1.00	23.51
20	49	CG1	ILE	A	688	34.173	2.557	84.174	1.00	26.92
	50	CG2	ILE	A	688	31.848	1.616	83.978	1.00	28.19
	51	CD1	ILE	A	688	34.884	1.237	84.088	1.00	31.87
25	52	N	ASN	A	689	30.505	3.704	86.674	1.00	25.92
	53	CA	ASN	A	689	29.118	3.713	87.138	1.00	27.71
	54	C	ASN	A	689	28.513	5.088	86.837	1.00	22.00
30	55	O	ASN	A	689	27.343	5.195	86.472	1.00	26.26
	56	CB	ASN	A	689	29.050	3.436	88.645	1.00	31.49
	57	CG	ASN	A	689	29.163	1.966	88.972	1.00	38.87
35	58	OD1	ASN	A	689	29.561	1.593	90.081	1.00	46.19
	59	ND2	ASN	A	689	28.778	1.116	88.023	1.00	36.32
	60	N	LEU	A	690	29.313	6.139	86.983	1.00	26.88
40	61	CA	LEU	A	690	28.811	7.491	86.715	1.00	25.43
	62	C	LEU	A	690	28.445	7.621	85.236	1.00	27.05
	63	O	LEU	A	690	27.384	8.139	84.895	1.00	26.07
45	64	CB	LEU	A	690	29.860	8.528	87.112	1.00	26.35
	65	CG	LEU	A	690	29.488	10.012	86.976	1.00	35.60
	66	CD1	LEU	A	690	30.409	10.836	87.880	1.00	36.71
50	67	CD2	LEU	A	690	29.595	10.475	85.522	1.00	30.46
	68	N	LEU	A	691	29.309	7.123	84.360	1.00	25.73
	69	CA	LEU	A	691	29.038	7.174	82.922	1.00	23.64
55	70	C	LEU	A	691	27.766	6.400	82.595	1.00	27.62
	71	O	LEU	A	691	26.990	6.810	81.738	1.00	22.81
	72	CB	LEU	A	691	30.209	6.586	82.128	1.00	24.64
55	73	CG	LEU	A	691	31.565	7.295	82.220	1.00	25.70
	74	CD1	LEU	A	691	32.610	6.538	81.381	1.00	21.63
	75	CD2	LEU	A	691	31.422	8.739	81.722	1.00	20.83
	76	N	MET	A	692	27.562	5.259	83.253	1.00	24.62

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	77	CA	MET	A	692	26.351	4.476	83.019	1.00	27.60
	78	C	MET	A	692	25.156	5.337	83.440	1.00	27.94
	79	O	MET	A	692	24.145	5.416	82.745	1.00	25.86
10	80	CB	MET	A	692	26.385	3.195	83.860	1.00	27.45
	81	CG	MET	A	692	25.197	2.289	83.686	1.00	39.52
	82	SD	MET	A	692	25.017	1.642	82.004	1.00	51.06
15	83	CE	MET	A	692	24.268	3.029	81.134	1.00	52.36
	84	N	SER	A	693	25.296	6.010	84.574	1.00	25.24
	85	CA	SER	A	693	24.216	6.835	85.083	1.00	31.97
20	86	C	SER	A	693	23.878	8.044	84.219	1.00	29.88
	87	O	SER	A	693	22.719	8.455	84.157	1.00	28.14
	88	CB	SER	A	693	24.531	7.313	86.508	1.00	38.05
25	89	OG	SER	A	693	25.623	8.222	86.526	1.00	43.01
	90	N	ILE	A	694	24.865	8.625	83.547	1.00	25.23
	91	CA	ILE	A	694	24.553	9.808	82.741	1.00	26.22
30	92	C	ILE	A	694	24.257	9.520	81.279	1.00	23.06
	93	O	ILE	A	694	24.031	10.442	80.504	1.00	24.41
	94	CB	ILE	A	694	25.669	10.875	82.813	1.00	22.83
35	95	CG1	ILE	A	694	26.984	10.307	82.265	1.00	22.20
	96	CG2	ILE	A	694	25.849	11.338	84.270	1.00	28.20
	97	CD1	ILE	A	694	28.060	11.373	82.014	1.00	22.62
40	98	N	GLU	A	695	24.257	8.242	80.899	1.00	26.89
	99	CA	GLU	A	695	23.969	7.876	79.517	1.00	21.93
	100	C	GLU	A	695	22.511	8.296	79.289	1.00	28.96
45	101	O	GLU	A	695	21.632	7.992	80.087	1.00	29.21
	102	CB	GLU	A	695	24.150	6.362	79.338	1.00	34.17
	103	CG	GLU	A	695	24.063	5.848	77.911	1.00	34.86
50	104	CD	GLU	A	695	25.240	6.232	77.021	1.00	45.46
	105	OE1	GLU	A	695	26.126	7.019	77.436	1.00	31.19
	106	OE2	GLU	A	695	25.275	5.730	75.873	1.00	49.30
55	107	N	PRO	A	696	22.242	9.037	78.215	1.00	32.33
	108	CA	PRO	A	696	20.865	9.469	77.961	1.00	34.70
	109	C	PRO	A	696	19.862	8.330	77.764	1.00	30.39
60	110	O	PRO	A	696	20.232	7.235	77.371	1.00	27.63
	111	CB	PRO	A	696	21.020	10.333	76.710	1.00	38.27
	112	CG	PRO	A	696	22.198	9.652	75.997	1.00	40.07
65	113	CD	PRO	A	696	23.141	9.561	77.173	1.00	34.72

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	114	N	ASP	A	697	18.588	8.613	78.037	1.00	38.27
	115	CA	ASP	A	697	17.516	7.632	77.863	1.00	35.46
	116	C	ASP	A	697	17.341	7.513	76.340	1.00	35.96
10	117	O	ASP	A	697	17.600	8.468	75.620	1.00	30.43
	118	CB	ASP	A	697	16.238	8.147	78.523	1.00	44.25
	119	CG	ASP	A	697	15.176	7.069	78.683	1.00	53.62
15	120	OD1	ASP	A	697	15.420	5.901	78.302	1.00	57.04
	121	OD2	ASP	A	697	14.085	7.398	79.203	1.00	61.97
	122	N	VAL	A	698	16.909	6.359	75.841	1.00	32.80
20	123	CA	VAL	A	698	16.766	6.195	74.393	1.00	34.66
	124	C	VAL	A	698	15.941	7.312	73.736	1.00	28.44
	125	O	VAL	A	698	14.937	7.775	74.266	1.00	30.11
25	126	CB	VAL	A	698	16.153	4.813	74.026	1.00	41.68
	127	CG1	VAL	A	698	14.649	4.830	74.237	1.00	38.06
	128	CG2	VAL	A	698	16.517	4.451	72.586	1.00	45.80
30	129	N	ILE	A	699	16.401	7.751	72.575	1.00	30.17
	130	CA	ILE	A	699	15.749	8.817	71.837	1.00	26.23
	131	C	ILE	A	699	14.912	8.250	70.696	1.00	28.40
35	132	O	ILE	A	699	15.381	7.393	69.954	1.00	22.17
	133	CB	ILE	A	699	16.809	9.774	71.240	1.00	28.58
	134	CG1	ILE	A	699	17.715	10.336	72.348	1.00	29.46
40	135	CG2	ILE	A	699	16.135	10.897	70.496	1.00	24.35
	136	CD1	ILE	A	699	16.979	11.118	73.395	1.00	37.93
	137	N	TYR	A	700	13.678	8.730	70.566	1.00	23.87
45	138	CA	TYR	A	700	12.788	8.305	69.488	1.00	27.94
	139	C	TYR	A	700	12.944	9.243	68.304	1.00	28.04
	140	O	TYR	A	700	13.238	10.427	68.474	1.00	24.24
50	141	CB	TYR	A	700	11.342	8.316	69.963	1.00	27.40
	142	CG	TYR	A	700	11.049	7.190	70.923	1.00	34.60
	143	CD1	TYR	A	700	11.300	7.331	72.284	1.00	37.81
55	144	CD2	TYR	A	700	10.584	5.960	70.462	1.00	38.29
	145	CE1	TYR	A	700	11.096	6.276	73.165	1.00	47.26
	146	CE2	TYR	A	700	10.374	4.893	71.337	1.00	39.38
55	147	CZ	TYR	A	700	10.634	5.062	72.687	1.00	41.71
	148	OH	TYR	A	700	10.434	4.024	73.569	1.00	52.51
	149	N	ALA	A	701	12.755	8.724	67.096	1.00	23.60
	150	CA	ALA	A	701	12.882	9.578	65.929	1.00	26.37

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	151	C	ALA	A	701	11.576	10.323	65.649	1.00	29.47
	152	O	ALA	A	701	11.579	11.354	64.970	1.00	28.14
	153	CB	ALA	A	701	13.272	8.762	64.709	1.00	27.79
10	154	N	GLY	A	702	10.474	9.811	66.187	1.00	29.99
	155	CA	GLY	A	702	9.179	10.419	65.925	1.00	32.21
	156	C	GLY	A	702	8.818	10.120	64.473	1.00	39.13
15	157	O	GLY	A	702	8.145	10.902	63.803	1.00	40.76
	158	N	HIS	A	703	9.278	8.970	63.983	1.00	38.38
	159	CA	HIS	A	703	9.042	8.558	62.602	1.00	46.41
20	160	C	HIS	A	703	7.638	7.980	62.347	1.00	47.68
	161	O	HIS	A	703	7.091	7.256	63.177	1.00	49.96
	162	CB	HIS	A	703	10.129	7.559	62.194	1.00	42.73
25	163	CG	HIS	A	703	9.978	7.034	60.803	1.00	48.58
	164	ND1	HIS	A	703	9.082	6.039	60.474	1.00	52.11
	165	CD2	HIS	A	703	10.589	7.388	59.649	1.00	46.18
30	166	CE1	HIS	A	703	9.151	5.800	59.177	1.00	50.15
	167	NE2	HIS	A	703	10.057	6.606	58.653	1.00	50.30
	168	N	ASP	A	704	7.079	8.306	61.181	1.00	51.90
35	169	CA	ASP	A	704	5.742	7.869	60.777	1.00	52.61
	170	C	ASP	A	704	5.506	6.363	60.863	1.00	54.82
	171	O	ASP	A	704	4.746	5.902	61.715	1.00	57.82
40	172	CB	ASP	A	704	5.453	8.356	59.359	1.00	52.84
	173	N	ASN	A	705	6.147	5.616	59.965	1.00	55.70
	174	CA	ASN	A	705	6.031	4.161	59.889	1.00	56.60
45	175	C	ASN	A	705	4.799	3.742	59.081	1.00	60.14
	176	O	ASN	A	705	4.906	2.984	58.109	1.00	61.18
	177	CB	ASN	A	705	5.979	3.551	61.295	1.00	57.02
50	178	N	THR	A	706	3.633	4.239	59.479	1.00	59.68
	179	CA	THR	A	706	2.384	3.911	58.794	1.00	60.50
	180	C	THR	A	706	2.420	4.213	57.289	1.00	61.78
55	181	O	THR	A	706	1.670	3.614	56.513	1.00	61.98
	182	CB	THR	A	706	1.226	4.662	59.451	1.00	57.03
	183	N	LYS	A	707	3.286	5.135	56.874	1.00	62.40
60	184	CA	LYS	A	707	3.386	5.488	55.459	1.00	64.42
	185	C	LYS	A	707	4.616	4.854	54.812	1.00	66.61
	186	O	LYS	A	707	5.571	4.477	55.502	1.00	64.83
65	187	CB	LYS	A	707	3.439	7.004	55.302	1.00	60.35

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
188	N	PRO	A	708	4.595	4.705	53.475	1.00	67.95
189	CA	PRO	A	708	5.704	4.119	52.713	1.00	69.09
190	C	PRO	A	708	6.924	5.047	52.748	1.00	68.98
191	O	PRO	A	708	6.891	6.153	52.205	1.00	70.54
192	CB	PRO	A	708	5.111	3.987	51.304	1.00	71.22
193	CG	PRO	A	708	3.600	3.904	51.570	1.00	69.09
194	CD	PRO	A	708	3.493	5.039	52.559	1.00	68.58
195	N	ASP	A	709	7.997	4.585	53.380	1.00	68.95
196	CA	ASP	A	709	9.220	5.371	53.510	1.00	68.41
197	C	ASP	A	709	9.961	5.612	52.197	1.00	65.11
198	O	ASP	A	709	10.416	4.666	51.556	1.00	67.29
199	CB	ASP	A	709	10.188	4.684	54.482	1.00	72.12
200	CG	ASP	A	709	9.584	4.452	55.861	1.00	74.27
201	OD1	ASP	A	709	8.401	4.798	56.074	1.00	77.63
202	OD2	ASP	A	709	10.302	3.918	56.733	1.00	75.63
203	N	THR	A	710	10.087	6.876	51.799	1.00	61.36
204	CA	THR	A	710	10.827	7.201	50.585	1.00	54.04
205	C	THR	A	710	12.256	7.499	51.026	1.00	53.38
206	O	THR	A	710	12.519	7.683	52.214	1.00	44.49
207	CB	THR	A	710	10.247	8.438	49.852	1.00	56.37
208	OG1	THR	A	710	10.381	9.603	50.674	1.00	58.14
209	CG2	THR	A	710	8.782	8.221	49.537	1.00	59.13
210	N	SER	A	711	13.182	7.535	50.079	1.00	47.04
211	CA	SER	A	711	14.566	7.807	50.412	1.00	48.03
212	C	SER	A	711	14.702	9.163	51.102	1.00	44.05
213	O	SER	A	711	15.368	9.278	52.129	1.00	41.23
214	CB	SER	A	711	15.415	7.760	49.146	1.00	50.15
215	OG	SER	A	711	15.267	6.499	48.508	1.00	63.32
216	N	SER	A	712	14.058	10.184	50.550	1.00	37.98
217	CA	SER	A	712	14.132	11.518	51.136	1.00	39.84
218	C	SER	A	712	13.389	11.627	52.472	1.00	37.46
219	O	SER	A	712	13.810	12.375	53.357	1.00	35.48
220	CB	SER	A	712	13.579	12.561	50.159	1.00	40.58
221	OG	SER	A	712	12.198	12.349	49.920	1.00	48.57
222	N	SER	A	713	12.285	10.900	52.630	1.00	36.47
223	CA	SER	A	713	11.548	10.979	53.890	1.00	34.65
224	C	SER	A	713	12.388	10.291	54.960	1.00	31.60

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	225	O	SER	A	713	12.459	10.737	56.102	1.00	28.24
	226	CB	SER	A	713	10.163	10.308	53.782	1.00	35.58
	227	OG	SER	A	713	10.266	8.900	53.711 1	1.00	43.95
10	228	N	LEU	A	714	13.040	9.207	54.574	1.00	27.90
	229	CA	LEU	A	714	13.897	8.469	55.490	1.00	29.29
	230	C	LEU	A	714	15.031	9.364	56.008	1.00	28.57
15	231	O	LEU	A	714	15.253	9.451	57.215	1.00	25.88
	232	CB	LEU	A	714	14.488	7.255	54.781	1.00	27.95
	233	CG	LEU	A	714	15.515	6.429	55.552	1.00	32.79
20	234	CD1	LEU	A	714	15.004	6.197	56.951	1.00	31.65
	235	CD2	LEU	A	714	15.783	5.110	54.823	1.00	36.96
	236	N	LEU	A	715	15.735	10.025	55.094	1.00	25.56
25	237	CA	LEU	A	715	16.832	10.915	55.482	1.00	24.24
	238	C	LEU	A	715	16.340	12.042	56.345	1.00	22.49
	239	O	LEU	A	715	16.992	12.398	57.317	1.00	21.35
30	240	CB	LEU	A	715	17.541	11.463	54.256	1.00	24.95
	241	CG	LEU	A	715	18.210	10.360	53.431	1.00	27.77
	242	CD1	LEU	A	715	18.781	10.946	52.146	1.00	27.06
35	243	CD2	LEU	A	715	19.300	9.695	54.259	1.00	32.37
	244	N	THR	A	716	15.179	12.598	56.004	1.00	21.24
	245	CA	THR	A	716	14.586	13.664	56.795	1.00	24.54
40	246	C	THR	A	716	14.306	13.159	58.207	1.00	24.54
	247	O	THR	A	716	14.552	13.864	59.181	1.00	21.07
	248	CB	THR	A	716	13.265	14.171	56.164	1.00	24.90
45	249	OG1	THR	A	716	13.561	14.873	54.948	1.00	26.56
	250	CG2	THR	A	716	12.520	15.088	57.125	1.00	23.35
	251	N	SER	A	717	13.776	11.945	58.322	1.00	19.11
50	252	CA	SER	A	717	13.508	11.381	59.635	1.00	21.51
	253	C	SER	A	717	14.815	11.112	60.389	1.00	19.84
	254	O	SER	A	717	14.860	11.270	61.619	1.00	21.66
55	255	CB	SER	A	717	12.706	10.077	59.527	1.00	24.02
	256	OG	SER	A	717	11.397	10.321	59.029	1.00	36.60
	257	N	LEU	A	718	15.866	10.687	59.683	1.00	18.47
55	258	CA	LEU	A	718	17.133	10.441	60.368	1.00	20.90
	259	C	LEU	A	718	17.738	11.766	60.828	1.00	20.84
	260	O	LEU	A	718	18.425	11.825	61.861	1.00	20.00
	261	CB	LEU	A	718	18.113	9.706	59.464	1.00	17.55

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
262	CG	LEU	A	718	17.770	8.242	59.191	1.00	19.20
263	CD1	LEU	A	718	18.704	7.721	58.127	1.00	20.15
264	CD2	LEU	A	718	17.902	7.418	60.467	1.00	19.08
265	N	ASN	A	719	17.498	12.832	60.070	1.00	17.81
266	CA	ASN	A	719	18.018	14.148	60.498	1.00	19.99
267	C	ASN	A	719	17.274	14.651	61.732	1.00	18.99
268	O	ASN	A	719	17.862	15.300	62.591	1.00	20.08
269	CB	ASN	A	719	17.910	15.208	59.392	1.00	22.67
270	CG	ASN	A	719	18.942	15.026	58.296	1.00	27.38
271	OD1	ASN	A	719	20.042	14.490	58.523	1.00	24.69
272	ND2	ASN	A	719	18.622	15.530	57.106	1.00	23.33
273	N	GLN	A	720	15.975	14.380	61.808	1.00	18.44
274	CA	GLN	A	720	15.165	14.785	62.966	1.00	21.61
275	C	GLN	A	720	15.693	14.023	64.186	1.00	23.93
276	O	GLN	A	720	15.832	14.582	65.273	1.00	18.25
277	CB	GLN	A	720	13.683	14.456	62.730	1.00	22.65
278	CG	GLN	A	720	12.817	14.620	63.963	1.00	26.41
279	CD	GLN	A	720	12.882	16.019	64.530	1.00	26.67
280	OE1	GLN	A	720	12.760	16.211	65.741	1.00	31.96
281	NE2	GLN	A	720	13.052	17.013	63.658	1.00	28.01
282	N	LEU	A	721	16.006	12.741	63.995	1.00	19.58
283	CA	LEU	A	721	16.568	11.942	65.084	1.00	17.13
284	C	LEU	A	721	17.924	12.545	65.476	1.00	16.29
285	O	LEU	A	721	18.228	12.690	66.662	1.00	19.55
286	CB	LEU	A	721	16.742	10.479	64.638	1.00	17.00
287	CG	LEU	A	721	17.378	9.549	65.673	1.00	19.10
288	CD1	LEU	A	721	16.508	9.497	66.942	1.00	18.65
289	CD2	LEU	A	721	17.536	8.145	65.037	1.00	17.08
290	N	GLY	A	722	18.724	12.896	64.476	1.00	16.83
291	CA	GLY	A	722	20.036	13.486	64.710	1.00	17.42
292	C	GLY	A	722	19.929	14.774	65.516	1.00	24.76
293	O	GLY	A	722	20.749	15.038	66.402	1.00	19.56
294	N	GLU	A	723	18.923	15.586	65.210	1.00	20.84
295	CA	GLU	A	723	18.709	16.848	65.951	1.00	22.88
296	C	GLU	A	723	18.408	16.526	67.410	1.00	23.92
297	O	GLU	A	723	18.896	17.195	68.328	1.00	23.22
298	CB	GLU	A	723	17.521	17.623	65.372	1.00	30.25

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	299	CG	GLU	A	723	17.240	18.998	66.018	1.00	27.93
	300	CD	GLU	A	723	18.083	20.112	65.417	1.00	37.81
	301	OE1	GLU	A	723	18.978	19.780	64.624	1.00	29.92
10	302	OE2	GLU	A	723	17.847	21.311	65.726	1.00	32.81
	303	N	ARG	A	724	17.597	15.496	67.640	1.00	17.75
	304	CA	ARG	A	724	17.258	15.112	69.007	1.00	19.86
15	305	C	ARG	A	724	18.445	14.490	69.735	1.00	18.81
	306	O	ARG	A	724	18.565	14.633	70.958	1.00	20.56
	307	CB	ARG	A	724	16.085	14.135	69.015	1.00	18.63
20	308	CG	ARG	A	724	14.820	14.733	68.421	1.00	24.16
	309	CD	ARG	A	724	13.713	13.709	68.362	1.00	28.88
	310	NE	ARG	A	724	12.531	14.280	67.730	1.00	27.71
25	311	CZ	ARG	A	724	11.330	13.726	67.739	1.00	32.19
	312	NH1	ARG	A	724	11.131	12.566	68.352	1.00	28.19
	313	NH2	ARG	A	724	10.315	14.360	67.162	1.00	35.89
30	314	N	GLN	A	725	19.296	13.770	69.009	1.00	19.77
	315	CA	GLN	A	725	20.474	13.188	69.634	1.00	19.30
	316	C	GLN	A	725	21.545	14.239	69.906	1.00	21.49
35	317	O	GLN	A	725	22.309	14.113	70.855	1.00	21.43
	318	CB	GLN	A	725	21.055	12.063	68.771	1.00	19.47
	319	CG	GLN	A	725	20.135	10.843	68.774	1.00	22.41
40	320	CD	GLN	A	725	20.746	9.633	68.092	1.00	30.53
	321	OE1	GLN	A	725	20.104	8.578	67.970	1.00	32.93
	322	NE2	GLN	A	725	21.987	9.770	67.647	1.00	27.09
45	323	N	LEU	A	726	21.592	15.284	69.085	1.00	21.82
	324	CA	LEU	A	726	22.573	16.347	69.288	1.00	22.79
	325	C	LEU	A	726	22.284	17.027	70.624	1.00	21.40
50	326	O	LEU	A	726	23.207	17.293	71.406	1.00	23.41
	327	CB	LEU	A	726	22.526	17.367	68.135	1.00	19.53
	328	CG	LEU	A	726	23.533	18.531	68.138	1.00	24.90
55	329	CD1	LEU	A	726	24.948	18.005	68.300	1.00	22.88
	330	CD2	LEU	A	726	23.421	19.325	66.812	1.00	20.28
	331	N	LEU	A	727	21.007	17.301	70.890	1.00	18.00
55	332	CA	LEU	A	727	20.623	17.906	72.156	1.00	19.91
	333	C	LEU	A	727	21.078	16.978	73.281	1.00	24.23
	334	O	LEU	A	727	21.678	17.402	74.274	1.00	19.07
	335	CB	LEU	A	727	19.105	18.065	72.247	1.00	21.64

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	336	CG	LEU	A	727	18.591	18.563	73.594	1.00	21.40
	337	CD1	LEU	A	727	19.256	19.906	73.912	1.00	26.36
	338	CD2	LEU	A	727	17.082	18.699	73.546	1.00	28.00
10	339	N	SER	A	728	20.783	15.695	73.106	1.00	21.94
	340	CA	SER	A	728	21.131	14.690	74.097	1.00	21.38
	341	C	SER	A	728	22.637	14.682	74.355	1.00	20.10
15	342	O	SER	A	728	23.066	14.611	75.512	1.00	22.32
	343	CB	SER	A	728	20.645	13.310	73.630	1.00	24.08
	344	OG	SER	A	728	20.719	12.380	74.689	1.00	30.43
20	345	N	VAL	A	729	23.433	14.741	73.297	1.00	18.72
	346	CA	VAL	A	729	24.891	14.781	73.415	1.00	20.27
	347	C	VAL	A	729	25.388	15.988	74.203	1.00	18.31
25	348	O	VAL	A	729	26.274	15.860	75.049	1.00	19.16
	349	CB	VAL	A	729	25.574	14.796	72.034	1.00	17.15
	350	CG1	VAL	A	729	27.060	15.147	72.164	1.00	20.31
30	351	CG2	VAL	A	729	25.453	13.395	71.407	1.00	21.83
	352	N	VAL	A	730	24.830	17.159	73.937	1.00	17.43
	353	CA	VAL	A	730	25.282	18.333	74.660	1.00	21.44
35	354	C	VAL	A	730	24.888	18.225	76.132	1.00	19.86
	355	O	VAL	A	730	25.678	18.584	76.993	1.00	21.47
	356	CB	VAL	A	730	24.725	19.630	74.038	1.00	20.22
40	357	CG1	VAL	A	730	25.210	20.849	74.834	1.00	21.24
	358	CG2	VAL	A	730	25.178	19.734	72.596	1.00	19.32
	359	N	LYS	A	731	23.686	17.727	76.427	1.00	17.73
45	360	CA	LYS	A	731	23.275	17.552	77.817	1.00	22.58
	361	C	LYS	A	731	24.186	16.546	78.517	1.00	23.23
	362	O	LYS	A	731	24.613	16.757	79.659	1.00	20.64
50	363	CB	LYS	A	731	21.808	17.121	77.911	1.00	23.07
	364	CG	LYS	A	731	20.850	18.296	77.646	1.00	25.92
	365	CD	LYS	A	731	19.388	18.009	78.016	1.00	37.08
55	366	CE	LYS	A	731	18.717	17.034	77.063	1.00	48.50
	367	NZ	LYS	A	731	17.247	16.901	77.346	1.00	49.18
	368	N	TRP	A	732	24.486	15.452	77.828	1.00	18.73
55	369	CA	TRP	A	732	25.383	14.437	78.364	1.00	21.37
	370	C	TRP	A	732	26.743	15.038	78.703	1.00	22.20
	371	O	TRP	A	732	27.293	14.772	79.770	1.00	23.93
	372	CB	TRP	A	732	25.552	13.321	77.334	1.00	21.47

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	373	CG	TRP	A	732	26.674	12.347	77.582	1.00	17.78
	374	CD1	TRP	A	732	26.728	11.348	78.528	1.00	20.71
	375	CD2	TRP	A	732	27.861	12.225	76.806	1.00	17.23
10	376	NE1	TRP	A	732	27.879	10.613	78.370	1.00	19.88
	377	CE2	TRP	A	732	28.593	11.130	77.318	1.00	19.41
	378	CE3	TRP	A	732	28.383	12.938	75.713	1.00	19.83
15	379	CZ2	TRP	A	732	29.824	10.726	76.771	1.00	18.15
	380	CZ3	TRP	A	732	29.612	12.533	75.165	1.00	20.23
	381	CH2	TRP	A	732	30.314	11.435	75.701	1.00	22.27
20	382	N	SER	A	733	27.274	15.872	77.811	1.00	20.68
	383	CA	SER	A	733	28.594	16.460	78.025	1.00	22.57
	384	C	SER	A	733	28.650	17.371	79.250	1.00	20.83
25	385	O	SER	A	733	29.701	17.523	79.843	1.00	22.59
	386	CB	SER	A	733	29.052	17.247	76.783	1.00	22.82
	387	OG	SER	A	733	28.287	18.431	76.611	1.00	27.11
30	388	N	LYS	A	734	27.522	17.976	79.619	1.00	20.76
	389	CA	LYS	A	734	27.495	18.878	80.769	1.00	25.82
	390	C	LYS	A	734	27.610	18.084	82.069	1.00	26.99
35	391	O	LYS	A	734	27.952	18.643	83.117	1.00	24.98
	392	CB	LYS	A	734	26.211	19.724	80.761	1.00	27.35
	393	CG	LYS	A	734	26.007	20.439	79.443	1.00	34.69
40	394	CD	LYS	A	734	25.400	21.833	79.600	1.00	44.84
	395	CE	LYS	A	734	24.047	21.812	80.278	1.00	49.64
	396	NZ	LYS	A	734	23.525	23.208	80.476	1.00	49.55
45	397	N	SER	A	735	27.325	16.786	82.003	1.00	23.17
	398	CA	SER	A	735	27.451	15.922	83.180	1.00	23.40
	399	C	SER	A	735	28.698	15.045	83.135	1.00	24.42
50	400	O	SER	A	735	29.010	14.345	84.110	1.00	21.97
	401	CB	SER	A	735	26.221	15.016	83.324	1.00	24.11
	402	OG	SER	A	735	25.066	15.769	83.629	1.00	29.58
55	403	N	LEU	A	736	29.421	15.085	82.015	1.00	19.77
	404	CA	LEU	A	736	30.613	14.246	81.835	1.00	21.02
	405	C	LEU	A	736	31.774	14.753	82.669	1.00	21.28
55	406	O	LEU	A	736	32.247	15.858	82.451	1.00	22.53
	407	CB	LEU	A	736	31.017	14.233	80.354	1.00	23.10
	408	CG	LEU	A	736	32.215	13.395	79.912	1.00	22.82
	409	CD1	LEU	A	736	31.963	11.915	80.168	1.00	22.40

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
410	CD2	LEU	A	736	32.443	13.639	78.412	1.00	20.94
411	N	PRO	A	737	32.285	13.930	83.595	1.00	22.85
412	CA	PRO	A	737	33.398	14.411	84.424	1.00	24.25
413	C	PRO	A	737	34.563	15.028	83.659	1.00	25.32
414	O	PRO	A	737	35.114	14.423	82.734	1.00	25.05
415	CB	PRO	A	737	33.790	13.163	85.219	1.00	24.36
416	CG	PRO	A	737	32.452	12.470	85.397	1.00	23.83
417	CD	PRO	A	737	31.958	12.535	83.947	1.00	20.46
418	N	GLY	A	738	34.911	16.253	84.053	1.00	25.15
419	CA	GLY	A	738	36.016	16.969	83.444	1.00	25.65
420	C	GLY	A	738	35.703	17.825	82.231	1.00	23.09
421	O	GLY	A	738	36.394	18.803	81.956	1.00	25.86
422	N	PHE	A	739	34.648	17.493	81.504	1.00	22.74
423	CA	PHE	A	739	34.363	18.252	80.296	1.00	23.63
424	C	PHE	A	739	34.018	19.717	80.536	1.00	22.42
425	O	PHE	A	739	34.537	20.591	79.856	1.00	21.78
426	CB	PHE	A	739	33.217	17.598	79.506	1.00	21.38
427	CG	PHE	A	739	33.129	18.065	78.077	1.00	20.80
428	CD1	PHE	A	739	34.130	17.715	77.165	1.00	22.81
429	CD2	PHE	A	739	32.063	18.851	77.642	1.00	24.10
430	CE1	PHE	A	739	34.072	18.134	75.848	1.00	24.39
431	CE2	PHE	A	739	31.998	19.278	76.313	1.00	19.38
432	CZ	PHE	A	739	33.001	18.918	75.423	1.00	23.48
433	N	ARG	A	740	33.147	19.979	81.508	1.00	22.15
434	CA	ARG	A	740	32.700	21.344	81.780	1.00	25.70
435	C	ARG	A	740	33.823	22.255	82.232	1.00	24.37
436	O	ARG	A	740	33.667	23.477	82.278	1.00	24.34
437	CB	ARG	A	740	31.615	21.352	82.851	1.00	23.04
438	CG	ARG	A	740	32.071	20.742	84.166	1.00	24.68
439	CD	ARG	A	740	31.094	21.087	85.281	1.00	25.40
440	NE	ARG	A	740	31.569	20.540	86.545	1.00	24.48
441	CZ	ARG	A	740	31.023	20.804	87.721	1.00	20.47
442	NH1	ARG	A	740	29.979	21.612	87.791	1.00	23.59
443	NH2	ARG	A	740	31.535	20.261	88.819	1.00	26.38
444	N	ASN	A	741	34.957	21.656	82.555	1.00	27.20
445	CA	ASN	A	741	36.100	22.409	83.029	1.00	23.55
446	C	ASN	A	741	37.024	22.889	81.918	1.00	26.53

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	447	O	ASN	A	741	37.922	23.694	82.170	27.16
	448	CB	ASN	A	741	36.828	21.571	84.063	32.06
	449	CG	ASN	A	741	35.926	21.211	85.230	33.85
10	450	OD1	ASN	A	741	36.120	20.201	85.899	37.94
	451	ND2	ASN	A	741	34.928	22.054	85.481	28.27
	452	N	LEU	A	742	36.806	22.402	80.698	22.63
	453	CA	LEU	A	742	37.572	22.859	79.547	22.51
15	454	C	LEU	A	742	36.961	24.201	79.206	19.73
	455	O	LEU	A	742	35.843	24.497	79.590	23.16
	456	CB	LEU	A	742	37.388	21.936	78.336	21.95
20	457	CG	LEU	A	742	37.803	20.486	78.573	20.73
	458	CD1	LEU	A	742	37.333	19.611	77.383	23.47
	459	CD2	LEU	A	742	39.318	20.415	78.768	22.85
	460	N	HIS	A	743	37.712	25.006	78.483	21.02
25	461	CA	HIS	A	743	37.248	26.319	78.056	25.86
	462	C	HIS	A	743	35.972	26.079	77.252	26.17
	463	O	HIS	A	743	35.873	25.074	76.559	23.09
30	464	CB	HIS	A	743	38.358	26.936	77.204	28.77
	465	CG	HIS	A	743	38.130	28.363	76.836	36.70
	466	ND1	HIS	A	743	37.179	28.753	75.921	34.14
	467	CD2	HIS	A	743	38.742	29.497	77.251	38.95
35	468	CE1	HIS	A	743	37.215	30.067	75.785	39.45
	469	NE2	HIS	A	743	38.155	30.542	76.582	39.37
	470	N	ILE	A	744	34.996	26.980	77.355	20.73
40	471	CA	ILE	A	744	33.743	26.827	76.623	27.73
	472	C	ILE	A	744	33.951	26.674	75.118	27.07
	473	O	ILE	A	744	33.264	25.875	74.461	24.14
45	474	CB	ILE	A	744	32.790	28.013	76.890	26.09
	475	CG1	ILE	A	744	32.515	28.111	78.389	32.88
	476	CG2	ILE	A	744	31.453	27.810	76.148	29.39
	477	CD1	ILE	A	744	31.940	26.858	78.979	39.72
50	478	N	ASP	A	745	34.888	27.432	74.554	24.97
	479	CA	ASP	A	745	35.140	27.317	73.126	27.70
	480	C	ASP	A	745	35.633	25.917	72.773	25.79
55	481	O	ASP	A	745	35.334	25.406	71.696	26.38
	482	CB	ASP	A	745	36.175	28.338	72.639	33.81
	483	CG	ASP	A	745	35.692	29.769	72.762	46.44

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	484	OD1	ASP	A	745	34.462	29.984	72.755	1.00	51.31
	485	OD2	ASP	A	745	36.548	30.683	72.829	1.00	50.96
	486	N	ASP	A	746	36.406	25.312	73.667	1.00	23.70
10	487	CA	ASP	A	746	36.904	23.971	73.418	1.00	22.43
	488	C	ASP	A	746	35.755	22.975	73.520	1.00	19.90
	489	O	ASP	A	746	35.672	22.049	72.712	1.00	22.60
15	490	CB	ASP	A	746	37.992	23.577	74.406	1.00	21.92
	491	CG	ASP	A	746	39.172	24.513	74.370	1.00	33.42
	492	OD1	ASP	A	746	39.421	25.130	73.300	1.00	34.56
20	493	OD2	ASP	A	746	39.862	24.610	75.408	1.00	39.54
	494	N	GLN	A	747	34.861	23.176	74.486	1.00	19.31
	495	CA	GLN	A	747	33.739	22.252	74.657	1.00	17.71
25	496	C	GLN	A	747	32.919	22.281	73.385	1.00	23.99
	497	O	GLN	A	747	32.563	21.238	72.852	1.00	19.91
	498	CB	GLN	A	747	32.846	22.655	75.826	1.00	19.37
30	499	CG	GLN	A	747	33.563	22.742	77.152	1.00	22.18
	500	CD	GLN	A	747	32.642	23.127	78.281	1.00	22.76
	501	OE1	GLN	A	747	33.052	23.798	79.230	1.00	25.01
35	502	NE2	GLN	A	747	31.397	22.675	78.212	1.00	18.79
	503	N	ILE	A	748	32.605	23.481	72.908	1.00	21.08
	504	CA	ILE	A	748	31.835	23.604	71.680	1.00	21.96
40	505	C	ILE	A	748	32.556	22.969	70.493	1.00	24.64
	506	O	ILE	A	748	31.942	22.218	69.732	1.00	23.28
	507	CB	ILE	A	748	31.527	25.087	71.368	1.00	25.55
45	508	CG1	ILE	A	748	30.603	25.642	72.445	1.00	22.21
	509	CG2	ILE	A	748	30.871	25.213	69.993	1.00	25.02
	510	CD1	ILE	A	748	30.292	27.138	72.308	1.00	26.31
50	511	N	THR	A	749	33.847	23.268	70.332	1.00	19.75
	512	CA	THR	A	749	34.645	22.716	69.240	1.00	20.18
	513	C	THR	A	749	34.678	21.177	69.271	1.00	19.01
55	514	O	THR	A	749	34.541	20.536	68.238	1.00	18.23
	515	CB	THR	A	749	36.104	23.229	69.301	1.00	24.15
	516	OG1	THR	A	749	36.104	24.656	69.166	1.00	26.23
55	517	CG2	THR	A	749	36.925	22.631	68.177	1.00	23.53
	518	N	LEU	A	750	34.864	20.583	70.450	1.00	17.46
	519	CA	LEU	A	750	34.899	19.117	70.541	1.00	19.07
	520	C	LEU	A	750	33.570	18.457	70.141	1.00	17.18

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	521	O	LEU	A	750	33.569	17.386	69.522	1.00	17.28
	522	CB	LEU	A	750	35.293	18.670	71.955	1.00	18.92
	523	CG	LEU	A	750	36.741	19.094	72.288	1.00	22.74
10	524	CD1	LEU	A	750	37.054	18.900	73.774	1.00	22.99
	525	CD2	LEU	A	750	37.674	18.281	71.444	1.00	20.48
	526	N	ILE	A	751	32.457	19.073	70.524	1.00	16.29
15	527	CA	ILE	A	751	31.136	18.544	70.148	1.00	23.76
	528	C	ILE	A	751	30.940	18.695	68.635	1.00	22.00
	529	O	ILE	A	751	30.462	17.777	67.966	1.00	17.05
20	530	CB	ILE	A	751	29.991	19.264	70.913	1.00	18.60
	531	CG1	ILE	A	751	30.014	18.842	72.388	1.00	22.25
	532	CG2	ILE	A	751	28.614	18.908	70.322	1.00	22.79
25	533	CD1	ILE	A	751	29.698	17.360	72.594	1.00	33.00
	534	N	GLN	A	752	31.311	19.848	68.085	1.00	21.43
	535	CA	GLN	A	752	31.144	20.031	66.643	1.00	23.26
30	536	C	GLN	A	752	32.038	19.105	65.824	1.00	22.82
	537	O	GLN	A	752	31.702	18.771	64.700	1.00	22.26
	538	CB	GLN	A	752	31.357	21.505	66.248	1.00	21.04
35	539	CG	GLN	A	752	30.346	22.408	66.965	1.00	26.41
	540	CD	GLN	A	752	30.410	23.867	66.541	1.00	34.88
	541	OE1	GLN	A	752	31.485	24.427	66.339	1.00	28.80
40	542	NE2	GLN	A	752	29.245	24.500	66.453	1.00	32.80
	543	N	TYR	A	753	33.171	18.680	66.381	1.00	21.10
	544	CA	TYR	A	753	34.060	17.765	65.657	1.00	23.73
45	545	C	TYR	A	753	33.590	16.333	65.756	1.00	21.41
	546	O	TYR	A	753	33.692	15.561	64.806	1.00	24.76
	547	CB	TYR	A	753	35.471	17.782	66.250	1.00	22.41
50	548	CG	TYR	A	753	36.339	18.964	65.885	1.00	21.14
	549	CD1	TYR	A	753	35.855	20.015	65.117	1.00	22.56
	550	CD2	TYR	A	753	37.666	19.006	66.295	1.00	25.54
55	551	CE1	TYR	A	753	36.683	21.093	64.759	1.00	27.58
	552	CE2	TYR	A	753	38.496	20.067	65.947	1.00	23.54
	553	CZ	TYR	A	753	38.002	21.104	65.181	1.00	22.36
55	554	OH	TYR	A	753	38.840	22.145	64.843	1.00	29.42
	555	N	SER	A	754	33.038	15.988	66.904	1.00	19.69
	556	CA	SER	A	754	32.699	14.594	67.147	1.00	21.05
	557	C	SER	A	754	31.265	14.109	67.119	1.00	20.67

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
558	O	SER	A	754	31.042	12.893	67.259	1.00	17.40
559	CB	SER	A	754	33.288	14.196	68.498	1.00	24.21
560	OG	SER	A	754	32.556	14.827	69.535	1.00	27.35
561	N	TRP	A	755	30.300	14.998	66.911	1.00	17.55
562	CA	TRP	A	755	28.912	14.547	66.960	1.00	21.93
563	C	TRP	A	755	28.620	13.345	66.055	1.00	18.91
564	O	TRP	A	755	27.956	12.409	66.486	1.00	20.07
565	CB	TRP	A	755	27.925	15.684	66.647	1.00	22.52
566	CG	TRP	A	755	28.003	16.222	65.257	1.00	23.08
567	CD1	TRP	A	755	28.859	17.175	64.791	1.00	28.21
568	CD2	TRP	A	755	27.217	15.803	64.141	1.00	24.51
569	NE1	TRP	A	755	28.655	17.379	63.445	1.00	25.19
570	CE2	TRP	A	755	27.651	16.548	63.022	1.00	26.64
571	CE3	TRP	A	755	26.189	14.869	63.979	1.00	25.75
572	CZ2	TRP	A	755	27.089	16.388	61.743	1.00	29.86
573	CZ3	TRP	A	755	25.630	14.707	62.707	1.00	32.59
574	CH2	TRP	A	755	26.083	15.465	61.608	1.00	30.85
575	N	MET	A	756	29.114	13.357	64.820	1.00	21.38
576	CA	MET	A	756	28.848	12.243	63.896	1.00	18.69
577	C	MET	A	756	29.439	10.939	64.415	1.00	23.20
578	O	MET	A	756	28.794	9.878	64.350	1.00	21.19
579	CB	MET	A	756	29.432	12.529	62.511	1.00	21.49
580	CG	MET	A	756	29.112	11.430	61.496	1.00	22.22
581	SD	MET	A	756	27.367	11.449	60.920	1.00	27.03
582	CE	MET	A	756	27.451	12.902	59.772	1.00	26.64
583	N	SER	A	757	30.675	11.013	64.899	1.00	19.23
584	CA	SER	A	757	31.344	9.845	65.451	1.00	22.32
585	C	SER	A	757	30.575	9.283	66.631	1.00	20.68
586	O	SER	A	757	30.376	8.078	66.718	1.00	21.09
587	CB	SER	A	757	32.759	10.190	65.911	1.00	23.54
588	OG	SER	A	757	33.562	10.611	64.826	1.00	31.88
589	N	LEU	A	758	30.150	10.149	67.548	1.00	20.06
590	CA	LEU	A	758	29.430	9.698	68.735	1.00	16.39
591	C	LEU	A	758	28.105	9.061	68.355	1.00	18.68
592	O	LEU	A	758	27.709	8.038	68.918	1.00	18.94
593	CB	LEU	A	758	29.147	10.880	69.675	1.00	14,15
594	CG	LEU	A	758	30.373	11.599	70.232	1.00	20.53

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	595	CD1	LEU	A	758	29.919	12.855	70.981	1.00	20.07
	596	CD2	LEU	A	758	31.121	10.656	71.186	1.00	24.11
	597	N	MET	A	759	27.410	9.674	67.404	1.00	18.42
10	598	CA	MET	A	759	26.125	9.149	67.001	1.00	19.21
	599	C	MET	A	759	26.209	7.828	66.242	1.00	19.93
	600	O	MET	A	759	25.363	6.949	66.456	1.00	23.09
15	601	CB	MET	A	759	25.364	10.197	66.193	1.00	21.20
	602	CG	MET	A	759	24.937	11.397	67.065	1.00	21.45
	603	SD	MET	A	759	23.950	12.587	66.168	1.00	25.97
20	604	CE	MET	A	759	23.941	13.961	67.348	1.00	26.52
	605	N	VAL	A	760	27.193	7.673	65.365	1.00	18.66
	606	CA	VAL	A	760	27.300	6.397	64.638	1.00	19.71
25	607	C	VAL	A	760	27.779	5.292	65.596	1.00	22.38
	608	O	VAL	A	760	27.409	4.127	65.448	1.00	18.63
	609	CB	VAL	A	760	28.262	6.492	63.417	1.00	20.60
30	610	CG1	VAL	A	760	29.708	6.659	63.860	1.00	22.90
	611	CG2	VAL	A	760	28.129	5.226	62.559	1.00	22.05
	612	N	PHE	A	761	28.597	5.672	66.572	1.00	18.16
35	613	CA	PHE	A	761	29.107	4.729	67.579	1.00	20.65
	614	C	PHE	A	761	27.907	4.256	68.419	1.00	21.25
	615	O	PHE	A	761	27.773	3.058	68.717	1.00	23.39
40	616	CB	PHE	A	761	30.166	5.441	68.447	1.00	19.84
	617	CG	PHE	A	761	31.100	4.502	69.206	1.00	22.22
	618	CD1	PHE	A	761	31.944	3.631	68.520	1.00	22.72
45	619	CD2	PHE	A	761	31.158	4.529	70.597	1.00	23.08
	620	CE1	PHE	A	761	32.834	2.802	69.200	1.00	23.74
	621	CE2	PHE	A	761	32.044	3.706	71.297	1.00	24.95
50	622	CZ	PHE	A	761	32.880	2.842	70.602	1.00	22.67
	623	N	GLY	A	762	27.041	5.196	68.803	1.00	18.00
	624	CA	GLY	A	762	25.851	4.861	69.564	1.00	19.15
55	625	C	GLY	A	762	24.928	3.957	68.761	1.00	19.60
	626	O	GLY	A	762	24.304	3.038	69.306	1.00	17.94
	627	N	LEU	A	763	24.815	4.241	67.465	1.00	18.18
55	628	CA	LEU	A	763	24.008	3.416	66.575	1.00	18.82
	629	C	LEU	A	763	24.562	1.994	66.611	1.00	20.32
	630	O	LEU	A	763	23.795	1.011	66.652	1.00	21.06
	631	CB	LEU	A	763	24.088	3.962	65.149	1.00	18.85

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5 632	CG	LEU	A	763	23.668	3.022	64.007	1.00	15.12
633	CD1	LEU	A	763	22.181	2.761	64.078	1.00	21.31
634	CD2	LEU	A	763	24.048	3.657	62.680	1.00	22.01
10 635	N	GLY	A	764	25.889	1.892	66.591	1.00	19.32
636	CA	GLY	A	764	26.546	0.596	66.609	1.00	22.15
637	C	GLY	A	764	26.182	-0.164	67.864	1.00	22.09
638	O	GLY	A	764	25.798	-1.351	67.826	1.00	18.52
15 639	N	TRP	A	765	26.279	0.520	68.998	1.00	18.65
640	CA	TRP	A	765	25.954	-0.118	70.265	1.00	21.70
641	C	TRP	A	765	24.485	-0.582	70.330	1.00	20.69
20 642	O	TRP	A	765	24.202	-1.710	70.730	1.00	20.73
643	CB	TRP	A	765	26.275	0.832	71.426	1.00	19.80
644	CG	TRP	A	765	25.985	0.232	72.766	1.00	20.60
645	CD1	TRP	A	765	24.895	0.450	73.543	1.00	26.35
25 646	CD2	TRP	A	765	26.765	-0.770	73.435	1.00	22.75
647	NE1	TRP	A	765	24.936	-0.354	74.660	1.00	25.80
648	CE2	TRP	A	765	26.076	-1.114	74.618	1.00	27.72
30 649	CE3	TRP	A	765	27.974	-1.408	73.145	1.00	24.76
650	CZ2	TRP	A	765	26.558	-2.080	75.522	1.00	28.33
651	CZ3	TRP	A	765	28.461	-2.372	74.045	1.00	25.79
652	CH2	TRP	A	765	27.747	-2.692	75.217	1.00	23.99
35 653	N	ARG	A	766	23.544	0.273	69.936	1.00	20.81
654	CA	ARG	A	766	22.136	-0.116	69.987	1.00	18.86
655	C	ARG	A	766	21.844	-1.288	69.048	1.00	18.44
40 656	O	ARG	A	766	21.066	-2.185	69.381	1.00	20.30
657	CB	ARG	A	766	21.223	1.061	69.624	1.00	18.28
658	CG	ARG	A	766	21.246	2.229	70.632	1.00	20.05
659	CD	ARG	A	766	20.179	3.260	70.256	1.00	25.08
45 660	NE	ARG	A	766	20.413	3.889	68.956	1.00	20.13
661	CZ	ARG	A	766	21.239	4.908	68.742	1.00	22.33
662	NH1	ARG	A	766	21.909	5.442	69.754	1.00	22.73
50 663	NH2	ARG	A	766	21.380	5.412	67.519	1.00	19.31
664	N	SER	A	767	22.469	-1.275	67.885	1.00	20.91
665	CA	SER	A	767	22.271	-2.340	66.899	1.00	18.59
666	C	SER	A	767	22.793	-3.660	67.473	1.00	24.76
55 667	O	SER	A	767	22.130	-4.692	67.406	1.00	19.96
668	CB	SER	A	767	23.002	-1.975	65.607	1.00	19.66

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	669	OG	SER	A	767	22.444	-0.786	65.077	1.00	23.01
	670	N	TYR	A	768	23.977	-3.595	68.067	1.00	20.64
	671	CA	TYR	A	768	24.604	-4.752	68.710	1.00	21.51
10	672	C	TYR	A	768	23.708	-5.300	69.831	1.00	20.49
	673	O	TYR	A	768	23.339	-6.481	69.841	1.00	20.85
	674	CB	TYR	A	768	25.963	-4.291	69.260	1.00	20.88
15	675	CG	TYR	A	768	26.629	-5.164	70.298	1.00	24.41
	676	CD1	TYR	A	768	26.882	-6.520	70.072	1.00	24.71
	677	CD2	TYR	A	768	27.126	-4.590	71.463	1.00	22.00
20	678	CE1	TYR	A	768	27.642	-7.273	70.993	1.00	21.58
	679	CE2	TYR	A	768	27.872	-5.325	72.370	1.00	21.74
	680	CZ	TYR	A	768	28.137	-6.656	72.125	1.00	24.16
25	681	OH	TYR	A	768	28.969	-7.309	73.000	1.00	22.86
	682	N	LYS	A	769	23.313	-4.427	70.751	1.00	19.61
	683	CA	LYS	A	769	22.500	-4.833	71.899	1.00	20.88
30	684	C	LYS	A	769	21.090	-5.323	71.636	1.00	25.83
	685	O	LYS	A	769	20.661	-6.320	72.222	1.00	23.20
	686	CB	LYS	A	769	22.402	-3.682	72.904	1.00	26.26
35	687	CG	LYS	A	769	23.682	-3.356	73.623	1.00	29.74
	688	CD	LYS	A	769	23.998	-4.345	74.756	1.00	34.33
	689	CE	LYS	A	769	23.010	-4.251	75.914	1.00	31.35
40	690	NZ	LYS	A	769	23.424	-5.118	77.078	1.00	27.64
	691	N	HIS	A	770	20.372	-4.627	70.762	1.00	20.34
	692	CA	HIS	A	770	18.968	-4.935	70.496	1.00	25.32
45	693	C	HIS	A	770	18.652	-5.887	69.353	1.00	24.30
	694	O	HIS	A	770	17.631	-6.572	69.382	1.00	23.64
	695	CB	HIS	A	770	18.204	-3.622	70.246	1.00	25.43
50	696	CG	HIS	A	770	18.239	-2.672	71.397	1.00	32.32
	697	ND1	HIS	A	770	17.517	-2.879	72.554	1.00	34.84
	698	CD2	HIS	A	770	18.920	-1.516	71.581	1.00	28.95
55	699	CE1	HIS	A	770	17.751	-1.889	73.398	1.00	36.65
	700	NE2	HIS	A	770	18.598	-1.049	72.833	1.00	35.04
	701	N	VAL	A	771	19.509	-5.934	68.341	1.00	24.39
55	702	CA	VAL	A	771	19.231	-6.795	67.202	1.00	25.76
	703	C	VAL	A	771	20.441	-7.614	66.787	1.00	24.92
	704	O	VAL	A	771	20.568	-8.008	65.639	1.00	27.56
	705	CB	VAL	A	771	18.687	-5.952	65.995	1.00	27.85

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5 706	CG1	VAL	A	771	17.295	-5.404	66.320	1.00	29.87
707	CG2	VAL	A	771	19.606	-4.767	65.718	1.00	28.77
708	N	SER	A	772	21.324	-7.883	67.745	1.00	22.68
10 709	CA	SER	A	772	22.532	-8.669	67.495	1.00	24.24
710	C	SER	A	772	23.352	-8.197	66.311	1.00	22.19
711	O	SER	A	772	24.033	-8.994	65.653	1.00	24.35
712	CB	SER	A	772	22.167	-10.153	67.332	1.00	22.79
15 713	OG	SER	A	772	21.539	-10.582	68.518	1.00	24.02
714	N	GLY	A	773	23.299	-6.886	66.062	1.00	20.76
715	CA	GLY	A	773	24.066	-6.290	64.982	1.00	21.80
20 716	C	GLY	A	773	23.555	-6.616	63.595	1.00	20.80
717	O	GLY	A	773	24.199	-6.274	62.604	1.00	25.34
718	N	GLN	A	774	22.386	-7.234	63.518	1.00	23.07
719	CA	GLN	A	774	21.845	-7.632	62.226	1.00	23.42
25 720	C	GLN	A	774	20.901	-6.638	61.538	1.00	25.60
721	O	GLN	A	774	20.414	-6.906	60.440	1.00	23.56
722	CB	GLN	A	774	21.174	-9.000	62.365	1.00	25.32
30 723	CG	GLN	A	774	22.103	-10.032	62.943	1.00	24.41
724	CD	GLN	A	774	23.443	-10.066	62.236	1.00	34.16
725	OE1	GLN	A	774	23.514	-10.285	61.030	1.00	40.94
726	NE2	GLN	A	774	24.517	-9.844	62.987	1.00	33.82
35 727	N	MET	A	775	20.625	-5.513	62.190	1.00	21.96
728	CA	MET	A	775	19.805	-4.447	61.603	1.00	22.20
729	C	MET	A	775	20.398	-3.172	62.206	1.00	24.08
40 730	O	MET	A	775	21.132	-3.256	63.188	1.00	21.84
731	CB	MET	A	775	18.332	-4.566	62.011	1.00	23.95
732	CG	MET	A	775	17.635	-5.838	61.531	1.00	28.07
733	SD	MET	A	775	15.873	-5.735	61.844	1.00	37.34
45 734	CE	MET	A	775	15.340	-7.409	61.263	1.00	37.01
735	N	LEU	A	776	20.115	-2.014	61.612	1.00	21.78
736	CA	LEU	A	776	20.621	-0.743	62.158	1.00	22.28
50 737	C	LEU	A	776	19.518	-0.144	63.016	1.00	20.07
738	O	LEU	A	776	18.489	0.318	62.520	1.00	21.05
739	CB	LEU	A	776	21.044	0.217	61.039	1.00	21.10
740	CG	LEU	A	776	22.256	-0.267	60.223	1.00	24.71
55 741	CD1	LEU	A	776	22.648	0.758	59.184	1.00	26.09
742	CD2	LEU	A	776	23.429	-0.534	61.159	1.00	23.43

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	743	N	TYR	A	777	19.733	-0.180	64.322	1.00	20.52
	744	CA	TYR	A	777	18.755	0.303	65.278	1.00	17.48
	745	C	TYR	A	777	18.967	1.804	65.547	1.00	21.46
10	746	O	TYR	A	777	19.525	2.184	66.565	1.00	18.14
	747	CB	TYR	A	777	18.902	-0.521	66.566	1.00	20.38
	748	CG	TYR	A	777	17.768	-0.416	67.572	1.00	22.57
15	749	CD1	TYR	A	777	17.608	0.717	68.373	1.00	22.04
	750	CD2	TYR	A	777	16.877	-1.474	67.748	1.00	25.77
	751	CE1	TYR	A	777	16.580	0.782	69.335	1.00	22.56
20	752	CE2	TYR	A	777	15.859	-1.421	68.693	1.00	25.86
	753	CZ	TYR	A	777	15.716	-0.299	69.485	1.00	23.25
	754	OH	TYR	A	777	14.721	-0.279	70.440	1.00	24.58
25	755	N	PHE	A	778	18.527	2.649	64.616	1.00	20.19
	756	CA	PHE	A	778	18.677	4.091	64.796	1.00	22.33
	757	C	PHE	A	778	17.888	4.572	66.019	1.00	19.77
30	758	O	PHE	A	778	18.369	5.373	66.817	1.00	20.69
	759	CB	PHE	A	778	18.233	4.843	63.526	1.00	17.81
	760	CG	PHE	A	778	19.170	4.685	62.380	1.00	19.78
35	761	CD1	PHE	A	778	19.038	3.633	61.485	1.00	26.89
	762	CD2	PHE	A	778	20.230	5.569	62.211	1.00	21.49
	763	CE1	PHE	A	778	19.963	3.474	60.432	1.00	24.89
40	764	CE2	PHE	A	778	21.151	5.413	61.168	1.00	21.92
	765	CZ	PHE	A	778	21.016	4.366	60.277	1.00	25.29
	766	N	ALA	A	779	16.672	4.079	66.169	1.00	18.84
45	767	CA	ALA	A	779	15.836	4.438	67.307	1.00	18.94
	768	C	ALA	A	779	14.808	3.318	67.390	1.00	23.24
	769	O	ALA	A	779	14.714	2.503	66.471	1.00	21.88
50	770	CB	ALA	A	779	15.151	5.785	67.063	1.00	19.00
	771	N	PRO	A	780	14.074	3.224	68.501	1.00	24.08
	772	CA	PRO	A	780	13.061	2.176	68.645	1.00	22.75
55	773	C	PRO	A	780	11.985	2.260	67.551	1.00	31.17
	774	O	PRO	A	780	11.405	1.242	67.163	1.00	27.19
	775	CB	PRO	A	780	12.506	2.451	70.039	1.00	23.42
55	776	CG	PRO	A	780	13.723	3.011	70.760	1.00	29.68
	777	CD	PRO	A	780	14.122	4.036	69.731	1.00	19.66
	778	N	ASP	A	781	11.728	3.465	67.045	1.00	24.25
	779	CA	ASP	A	781	10.722	3.643	65.995	1.00	30.35

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	780	C	ASP	A	781	11.345	3.803	64.608	1.00	28.45
	781	O	ASP	A	781	10.666	4.154	63.631	1.00	31.54
	782	CB	ASP	A	781	9.856	4.854	66.328	1.00	33.03
10	783	CG	ASP	A	781	10.648	6.149	66.354	1.00	42.61
	784	OD1	ASP	A	781	11.799	6.152	66.847	1.00	37.30
	785	OD2	ASP	A	781	10.105	7.175	65.899	1.00	39.66
15	786	N	LEU	A	782	12.640	3.528	64.518	1.00	25.42
	787	CA	LEU	A	782	13.352	3.654	63.264	1.00	23.61
	788	C	LEU	A	782	14.483	2.619	63.221	1.00	25.27
20	789	O	LEU	A	782	15.635	2.899	63.548	1.00	21.60
	790	CB	LEU	A	782	13.907	5.072	63.134	1.00	25.81
	791	CG	LEU	A	782	14.296	5.483	61.718	1.00	26.41
25	792	CD1	LEU	A	782	13.086	5.260	60.823	1.00	37.20
	793	CD2	LEU	A	782	14.693	6.947	61.682	1.00	23.25
	794	N	ILE	A	783	14.117	1.401	62.844	1.00	20.00
30	795	CA	ILE	A	783	15.048	0.298	62.742	1.00	21.82
	796	C	ILE	A	783	15.144	-0.054	61.258	1.00	26.37
	797	O	ILE	A	783	14.125	-0.343	60.640	1.00	27.10
35	798	CB	ILE	A	783	14.500	-0.924	63.496	1.00	19.86
	799	CG1	ILE	A	783	14.240	-0.558	64.957	1.00	23.93
	800	CG2	ILE	A	783	15.491	-2.086	63.374	1.00	26.69
40	801	CD1	ILE	A	783	13.358	-1.543	65.718	1.00	22.62
	802	N	LEU	A	784	16.346	-0.041	60.690	1.00	24.00
	803	CA	LEU	A	784	16.496	-0.369	59.277	1.00	30.39
45	804	C	LEU	A	784	17.146	-1.717	58.979	1.00	28.22
	805	O	LEU	A	784	18.156	-2.095	59.583	1.00	27.38
	806	CB	LEU	A	784	17.296	0.715	58.547	1.00	27.74
50	807	CG	LEU	A	784	16.753	2.148	58.588	1.00	33.96
	808	CD1	LEU	A	784	17.619	3.030	57.678	1.00	30.69
	809	CD2	LEU	A	784	15.306	2.182	58.142	1.00	33.34
55	810	N	ASN	A	785	16.545	-2.421	58.022	1.00	37.87
	811	CA	ASN	A	785	17.041	-3.708	57.537	1.00	34.28
	812	C	ASN	A	785	17.310	-3.491	56.050	1.00	40.43
55	813	O	ASN	A	785	16.947	-2.442	55.492	1.00	32.88
	814	CB	ASN	A	785	15.998	-4.814	57.720	1.00	43.78
	815	CG	ASN	A	785	14.679	-4.482	57.058	1.00	39.05
	816	OD1	ASN	A	785	14.644	-4.013	55.922	1.00	56.25

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	817	ND2	ASN	A	785	13.584	-4.740	57.758	1.00	55.74
	818	N	GLU	A	786	17.945	-4.475	55.419	1.00	37.34
	819	CA	GLU	A	786	18.290	-4.406	54.001	1.00	41.84
10	820	C	GLU	A	786	17.137	-3.983	53.103	1.00	36.02
	821	O	GLU	A	786	17.332	-3.187	52.190	1.00	37.52
	822	CB	GLU	A	786	18.829	-5.753	53.508	1.00	43.26
15	823	CG	GLU	A	786	20.141	-6.218	54.140	1.00	53.06
	824	CD	GLU	A	786	19.987	-6.714	55.569	1.00	52.18
	825	OE1	GLU	A	786	18.877	-6.622	56.135	1.00	55.65
20	826	OE2	GLU	A	786	20.990	-7.206	56.128	1.00	59.59
	827	N	GLN	A	787	15.945	-4.515	53.360	1.00	37.37
	828	CA	GLN	A	787	14.757	-4.194	52.563	1.00	41.31
25	829	C	GLN	A	787	14.403	-2.705	52.523	1.00	44.67
	830	O	GLN	A	787	13.863	-2.214	51.529	1.00	39.36
	831	CB	GLN	A	787	13.541	-4.954	53.094	1.00	39.63
30	832	CG	GLN	A	787	13.659	-6.470	53.044	1.00	54.67
	833	CD	GLN	A	787	12.516	-7.161	53.765	1.00	54.04
	834	OE1	GLN	A	787	11.359	-7.095	53.343	1.00	65.04
35	835	NE2	GLN	A	787	12.835	-7.819	54.871	1.00	58.37
	836	N	ARG	A	788	14.709	-1.989	53.600	1.00	42.38
	837	CA	ARG	A	788	14.379	-0.570	53.680	1.00	46.01
40	838	C	ARG	A	788	15.474	0.355	53.157	1.00	44.06
	839	O	ARG	A	788	15.307	1.576	53.123	1.00	43.28
	840	CB	ARG	A	788	14.020	-0.219	55.129	1.00	45.62
45	841	CG	ARG	A	788	12.956	-1.149	55.694	1.00	51.99
	842	CD	ARG	A	788	12.554	-0.827	57.121	1.00	54.00
	843	NE	ARG	A	788	11.834	0.440	57.238	1.00	62.20
50	844	CZ	ARG	A	788	11.303	0.893	58.372	1.00	62.82
	845	NH1	ARG	A	788	11.411	0.184	59.490	1.00	63.08
	846	NH2	ARG	A	788	10.659	2.052	58.391	1.00	64.33
55	847	N	MET	A	789	16.589	-0.226	52.738	1.00	42.60
	848	CA	MET	A	789	17.690	0.563	52.207	1.00	44.82
	849	C	MET	A	789	17.687	0.382	50.697	1.00	44.81
55	850	O	MET	A	789	18.545	-0.303	50.143	1.00	41.79
	851	CB	MET	A	789	19.013	0.072	52.791	1.00	47.11
	852	CG	MET	A	789	19.047	0.097	54.307	1.00	38.54
	853	SD	MET	A	789	20.519	-0.711	54.954	1.00	40.15

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
854	CE	MET	A	789	20.192	-0.603	56.713	1.00	40.02
855	N	LYS	A	790	16.706	0.990	50.040	1.00	45.90
856	CA	LYS	A	790	16.575	0.879	48.591	1.00	49.64
857	C	LYS	A	790	17.686	1.632	47.883	1.00	52.38
858	O	LYS	A	790	18.423	1.065	47.073	1.00	56.13
859	CB	LYS	A	790	15.225	1.435	48.148	1.00	52.46
860	CG	LYS	A	790	14.047	0.799	48.844	1.00	50.21
861	CD	LYS	A	790	12.752	1.440	48.405	1.00	55.50
862	CE	LYS	A	790	11.583	0.875	49.176	1.00	54.17
863	NZ	LYS	A	790	10.334	1.600	48.845	1.00	57.04
864	N	GLU	A	791	17.782	2.920	48.194	1.00	54.04
865	CA	GLU	A	791	18.780	3.817	47.621	1.00	54.00
866	C	GLU	A	791	20.162	3.174	47.656	1.00	52.73
867	O	GLU	A	791	20.689	2.887	48.728	1.00	52.98
868	CB	GLU	A	791	18.792	5.116	48.427	1.00	61.18
869	CG	GLU	A	791	19.609	6.246	47.844	1.00	67.64
870	CD	GLU	A	791	19.632	7.444	48.769	1.00	74.88
871	OE1	GLU	A	791	18.547	7.856	49.241	1.00	78.04
872	OE2	GLU	A	791	20.733	7.979	49.017	1.00	77.72
873	N	SER	A	792	20.755	2.947	46.490	1.00	47.20
874	CA	SER	A	792	22.074	2.326	46.439	1.00	47.93
875	C	SER	A	792	23.177	3.113	47.168	1.00	45.20
876	O	SER	A	792	24.041	2.507	47.813	1.00	41.96
877	CB	SER	A	792	22.475	2.064	44.979	1.00	47.55
878	OG	SER	A	792	22.355	3.235	44.193	1.00	54.54
879	N	SER	A	793	23.153	4.448	47.077	1.00	41.56
880	CA	SER	A	793	24.175	5.262	47.746	1.00	34.71
881	C	SER	A	793	24.018	5.190	49.268	1.00	33.35
882	O	SER	A	793	25.009	5.091	49.988	1.00	30.89
883	CB	SER	A	793	24.100	6.728	47.289	1.00	36.41
884	OG	SER	A	793	22.859	7.318	47.626	1.00	41.06
885	N	PHE	A	794	22.774	5.227	49.739	1.00	32.63
886	CA	PHE	A	794	22.492	5.165	51.170	1.00	35.71
887	C	PHE	A	794	22.762	3.762	51.725	1.00	35.32
888	O	PHE	A	794	23.256	3.613	52.839	1.00	33.54
889	CB	PHE	A	794	21.044	5.564	51.447	1.00	42.64
890	CG	PHE	A	794	20.716	5.627	52.906	1.00	46.25

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	891	CD1	PHE	A	794	21.441	6.457	53.751	1.00	47.24
	892	CD2	PHE	A	794	19.714	4.832	53.442	1.00	50.84
	893	CE1	PHE	A	794	21.176	6.495	55.118	1.00	52.49
10	894	CE2	PHE	A	794	19.441	4.862	54.805	1.00	52.13
	895	CZ	PHE	A	794	20.177	5.696	55.643	1.00	44.92
	896	N	TYR	A	795	22.435	2.738	50.942	1.00	31.90
15	897	CA	TYR	A	795	22.687	1.355	51.356	1.00	28.99
	898	C	TYR	A	795	24.184	1.203	51.510	1.00	25.10
	899	O	TYR	A	795	24.671	0.609	52.465	1.00	29.55
20	900	CB	TYR	A	795	22.183	0.378	50.287	1.00	37.34
	901	CG	TYR	A	795	22.478	-1.079	50.578	1.00	40.29
	902	CD1	TYR	A	795	21.891	-1.730	51.666	1.00	40.54
25	903	CD2	TYR	A	795	23.331	-1.810	49.753	1.00	42.80
	904	CE1	TYR	A	795	22.145	-3.068	51.923	1.00	42.21
	905	CE2	TYR	A	795	23.592	-3.154	50.001	1.00	45.44
30	906	CZ	TYR	A	795	22.992	-3.779	51.087	1.00	44.14
	907	OH	TYR	A	795	23.225	-5.116	51.323	1.00	48.25
	908	N	SER	A	796	24.937	1.757	50.571	1.00	24.54
35	909	CA	SER	A	796	26.373	1.631	50.665	1.00	25.44
	910	C	SER	A	796	26.866	2.323	51.932	1.00	28.08
	911	O	SER	A	796	27.807	1.855	52.569	1.00	31.55
40	912	CB	SER	A	796	27.053	2.239	49.439	1.00	32.47
	913	OG	SER	A	796	28.460	2.133	49.564	1.00	43.41
	914	N	LEU	A	797	26.239	3.438	52.295	1.00	25.12
45	915	CA	LEU	A	797	26.665	4.141	53.503	1.00	25.95
	916	C	LEU	A	797	26.302	3.314	54.736	1.00	27.16
	917	O	LEU	A	797	27.044	3.292	55.716	1.00	29.13
50	918	CB	LEU	A	797	26.010	5.520	53.603	1.00	32.01
	919	CG	LEU	A	797	26.631	6.398	54.704	1.00	30.49
	920	CD1	LEU	A	797	28.039	6.772	54.291	1.00	36.98
55	921	CD2	LEU	A	797	25.822	7.646	54.917	1.00	32.88
	922	N	CYS	A	798	25.152	2.650	54.695	1.00	26.93
	923	CA	CYS	A	798	24.736	1.811	55.810	1.00	28.14
55	924	C	CYS	A	798	25.681	0.634	56.017	1.00	24.65
	925	O	CYS	A	798	25.953	0.253	57.157	1.00	25.73
	926	CB	CYS	A	798	23.306	1.308	55.607	1.00	24.73
	927	SG	CYS	A	798	22.054	2.594	55.812	1.00	32.75

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5 928	N	LEU	A	799	26.181	0.054	54.925	1.00	25.25
929	CA	LEU	A	799	27.124	-1.059	55.034	1.00	26.29
930	C	LEU	A	799	28.387	-0.603	55.732	1.00	27.01
10 931	O	LEU	A	799	29.047	-1.374	56.441	1.00	27.73
932	CB	LEU	A	799	27.492	-1.602	53.654	1.00	28.72
933	CG	LEU	A	799	26.395	-2.303	52.861	1.00	35.76
934	CD1	LEU	A	799	26.980	-2.774	51.524	1.00	38.62
15 935	CD2	LEU	A	799	25.859	-3.485	53.660	1.00	34.72
936	N	THR	A	800	28.743	0.655	55.501	1.00	28.68
937	CA	THR	A	800	29.918	1.242	56.125	1.00	27.55
20 938	C	THR	A	800	29.636	1.394	57.612	1.00	20.19
939	O	THR	A	800	30.487	1.090	58.447	1.00	28.87
940	CB	THR	A	800	30.222	2.620	55.503	1.00	37.30
941	OG1	THR	A	800	30.660	2.421	54.153	1.00	34.67
25 942	CG2	THR	A	800	31.290	3.374	56.302	1.00	32.14
943	N	MET	A	801	28.442	1.871	57.935	1.00	20.28
944	CA	MET	A	801	28.063	2.042	59.333	1.00	23.80
30 945	C	MET	A	801	27.990	0.679	60.017	1.00	25.24
946	O	MET	A	801	28.380	0.535	61.173	1.00	23.42
947	CB	MET	A	801	26.705	2.750	59.439	1.00	23.19
948	CG	MET	A	801	26.745	4.207	58.953	1.00	25.74
35 949	SD	MET	A	801	25.204	5.075	59.342	1.00	29.64
950	CE	MET	A	801	24.118	4.431	58.116	1.00	40.66
40 951	N	TRP	A	802	27.512	-0.318	59.280	1.00	27.17
952	CA	TRP	A	802	27.352	-1.674	59.804	1.00	27.11
953	C	TRP	A	802	28.642	-2.297	60.328	1.00	28.77
954	O	TRP	A	802	28.617	-3.235	61.132	1.00	26.96
45 955	CB	TRP	A	802	26.764	-2.588	58.733	1.00	27.64
956	CG	TRP	A	802	25.504	-3.273	59.178	1.00	29.69
957	CD1	TRP	A	802	25.309	-3.977	60.341	1.00	24.68
958	CD2	TRP	A	802	24.261	-3.308	58.475	1.00	27.66
50 959	NE1	TRP	A	802	24.019	-4.441	60.398	1.00	31.31
960	CE2	TRP	A	802	23.352	-4.047	59.268	1.00	31.04
961	CE3	TRP	A	802	23.822	-2.785	57.248	1.00	37.29
55 962	CZ2	TRP	A	802	22.028	-4.278	58.874	1.00	31.47
963	CZ3	TRP	A	802	22.503	-3.012	56.855	1.00	25.61
964	CH2	TRP	A	802	21.622	-3.754	57.670	1.00	33.86

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	965	N	GLN	A	803	29.772	-1.775	59.870	1.00	27.01
	966	CA	GLN	A	803	31.066	-2.280	60.304	1.00	29.15
	967	C	GLN	A	803	31.242	-2.199	61.810	1.00	27.44
10	968	O	GLN	A	803	31.895	-3.052	62.408	1.00	26.00
	969	CB	GLN	A	803	32.190	-1.492	59.648	1.00	27.84
	970	CG	GLN	A	803	32.293	-1.680	58.156	1.00	27.53
15	971	CD	GLN	A	803	33.392	-0.813	57.564	1.00	37.98
	972	OE1	GLN	A	803	33.273	0.414	57.508	1.00	41.49
	973	NE2	GLN	A	803	34.477	-1.446	57.145	1.00	37.86
20	974	N	ILE	A	804	30.683	-1.163	62.424	1.00	23.42
	975	CA	ILE	A	804	30.825	-1.016	63.861	1.00	25.19
	976	C	ILE	A	804	30.106	-2.116	64.658	1.00	22.21
25	977	O	ILE	A	804	30.737	-2.795	65.467	1.00	28.86
	978	CB	ILE	A	804	30.353	0.379	64.330	1.00	25.31
	979	CG1	ILE	A	804	31.085	1.467	63.531	1.00	27.19
30	980	CG2	ILE	A	804	30.639	0.537	65.826	1.00	29.31
	981	CD1	ILE	A	804	30.774	2.893	63.988	1.00	29.28
	982	N	PRO	A	805	28.790	-2.309	64.455	1.00	22.89
35	983	CA	PRO	A	805	28.092	-3.366	65.211	1.00	26.67
	984	C	PRO	A	805	28.769	-4.716	64.986	1.00	25.60
	985	O	PRO	A	805	28.815	-5.568	65.879	1.00	25.13
40	986	CB	PRO	A	805	26.686	-3.353	64.602	1.00	22.17
	987	CG	PRO	A	805	26.531	-1.937	64.165	1.00	33.89
	988	CD	PRO	A	805	27.852	-1.659	63.522	1.00	25.28
45	989	N	GLN	A	806	29.287	-4.903	63.773	1.00	29.12
	990	CA	GLN	A	806	29.971	-6.144	63.416	1.00	28.65
	991	C	GLN	A	806	31.202	-6.364	64.259	1.00	30.22
50	992	O	GLN	A	806	31.441	-7.478	64.714	1.00	28.51
	993	CB	GLN	A	806	30.348	-6.156	61.928	1.00	33.89
	994	CG	GLN	A	806	29.136	-6.069	61.024	1.00	40.04
55	995	CD	GLN	A	806	28.130	-7.161	61.297	1.00	51.23
	996	OE1	GLN	A	806	27.651	-7.316	62.425	1.00	56.13
	997	NE2	GLN	A	806	27.787	-7.923	60.260	1.00	58.14
55	998	N	GLU	A	807	31.986	-5.312	64.477	1.00	25.11
	999	CA	GLU	A	807	33.174	-5.446	65.299	1.00	25.25
	1000	C	GLU	A	807	32.775	-5.606	66.742	1.00	21.49
	1001	O	GLU	A	807	33.476	-6.286	67.484	1.00	25.66

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1002	CB	GLU	A	807	34.120	-4.249	65.122	1.00	28.40
1003	CG	GLU	A	807	34.779	-4.252	63.762	1.00	41.59
1004	CD	GLU	A	807	35.673	-5.480	63.565	1.00	49.95
1005	OE1	GLU	A	807	36.146	-6.046	64.576	1.00	44.78
1006	OE2	GLU	A	807	35.920	-5.871	62.401	1.00	51.07
1007	N	PHE	A	808	31.651	-4.992	67.131	1.00	24.33
1008	CA	PHE	A	808	31.143	-5.090	68.500	1.00	26.06
1009	C	PHE	A	808	30.783	-6.533	68.780	1.00	26.07
1010	O	PHE	A	808	31.086	-7.052	69.845	1.00	22.03
1011	CB	PHE	A	808	29.905	-4.197	68.722	1.00	22.64
1012	CG	PHE	A	808	30.241	-2.741	68.942	1.00	21.70
1013	CD1	PHE	A	808	31.554	-2.306	68.890	1.00	24.72
1014	CD2	PHE	A	808	29.239	-1.814	69.223	1.00	24.00
1015	CE1	PHE	A	808	31.881	-0.961	69.116	1.00	28.45
1016	CE2	PHE	A	808	29.546	-0.471	69.451	1.00	23.16
1017	CZ	PHE	A	808	30.872	-0.045	69.398	1.00	26.38
1018	N	VAL	A	809	30.146	-7.176	67.806	1.00	26.08
1019	CA	VAL	A	809	29.762	-8.588	67.937	1.00	24.64
1020	C	VAL	A	809	31.002	-9.470	67.997	1.00	26.29
1021	O	VAL	A	809	31.119	-10.337	68.866	1.00	28.56
1022	CB	VAL	A	809	28.893	-9.023	66.744	1.00	28.11
1023	CG1	VAL	A	809	28.782	-10.541	66.691	1.00	30.55
1024	CG2	VAL	A	809	27.514	-8.415	66.877	1.00	29.17
1025	N	LYS	A	810	31.934	-9.242	67.074	1.00	22.16
1026	CA	LYS	A	810	33.163	-10.023	66.997	1.00	28.14
1027	C	LYS	A	810	34.005	-9.923	68.275	1.00	29.30
1028	O	LYS	A	810	34.468	-10.931	68.823	1.00	29.13
1029	CB	LYS	A	810	33.970	-9.547	65.785	1.00	31.67
1030	CG	LYS	A	810	35.211	-10.349	65.433	1.00	41.13
1031	CD	LYS	A	810	35.952	-9.686	64.256	1.00	46.76
1032	CE	LYS	A	810	35.028	-9.495	63.053	1.00	48.50
1033	NZ	LYS	A	810	35.669	-8.774	61.916	1.00	53.84
1034	N	LEU	A	811	34.203	-8.704	68.758	1.00	29.04
1035	CA	LEU	A	811	34.997	-8.495	69.962	1.00	27.03
1036	C	LEU	A	811	34.227	-8.671	71.271	1.00	24.56
1037	O	LEU	A	811	34.834	-8.749	72.344	1.00	25.98
1038	CB	LEU	A	811	35.613	-7.086	69.942	1.00	30.03

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1039	CG	LEU	A	811	36.682	-6.756	68.897	1.00	36.08
	1040	CD1	LEU	A	811	37.157	-5.327	69.075	1.00	28.22
	1041	CD2	LEU	A	811	37.849	-7.707	69.059	1.00	33.46
10	1042	N	GLN	A	812	32.901	-8.734	71.184	1.00	24.63
	1043	CA	GLN	A	812	32.052	-8.840	72.366	1.00	24.29
	1044	C	GLN	A	812	32.351	-7.707	73.363	1.00	28.28
15	1045	O	GLN	A	812	32.608	-7.935	74.553	1.00	26.02
	1046	CB	GLN	A	812	32.202	-10.214	73.030	1.00	31.81
	1047	CG	GLN	A	812	31.752	-11.335	72.115	1.00	34.45
20	1048	CD	GLN	A	812	31.604	-12.687	72.810	1.00	43.12
	1049	OE1	GLN	A	812	31.282	-13.693	72.162	1.00	48.46
	1050	NE2	GLN	A	812	31.825	-12.720	74.117	1.00	38.30
25	1051	N	VAL	A	813	32.314	-6.479	72.851	1.00	23.00
	1052	CA	VAL	A	813	32.547	-5.274	73.659	1.00	23.27
	1053	C	VAL	A	813	31.539	-5.173	74.804	1.00	20.62
30	1054	O	VAL	A	813	30.342	-5.422	74.631	1.00	24.25
	1055	CB	VAL	A	813	32.452	-4.002	72.776	1.00	22.34
	1056	CG1	VAL	A	813	32.527	-2.735	73.626	1.00	22.21
35	1057	CG2	VAL	A	813	33.564	-4.017	71.777	1.00	20.16
	1058	N	SER	A	814	32.033	-4.814	75.984	1.00	21.62
	1059	CA	SER	A	814	31.168	-4.708	77.141	1.00	22.92
40	1060	C	SER	A	814	30.636	-3.294	77.308	1.00	21.08
	1061	O	SER	A	814	31.191	-2.345	76.763	1.00	22.56
	1062	CB	SER	A	814	31.931	-5.094	78.406	1.00	23.84
45	1063	OG	SER	A	814	32.977	-4.161	78.643	1.00	27.14
	1064	N	GLN	A	815	29.549	-3.174	78.057	1.00	22.79
	1065	CA	GLN	A	815	28.938	-1.882	78.332	1.00	26.53
50	1066	C	GLN	A	815	29.995	-0.959	78.945	1.00	24.03
	1067	O	GLN	A	815	30.083	0.209	78.590	1.00	23.00
	1068	CB	GLN	A	815	27.757	-2.077	79.304	1.00	26.89
55	1069	CG	GLN	A	815	27.053	-0.812	79.802	1.00	37.27
	1070	CD	GLN	A	815	26.399	-0.002	78.700	1.00	46.40
	1071	OE1	GLN	A	815	27.072	0.686	77.927	1.00	49.69
55	1072	NE2	GLN	A	815	25.073	-0.085	78.618	1.00	48.97
	1073	N	GLU	A	816	30.806	-1.498	79.853	1.00	24.42
	1074	CA	GLU	A	816	31.844	-0.706	80.527	1.00	24.69
	1075	C	GLU	A	816	32.909	-0.216	79.555	1.00	21.73

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1076	O	GLU	A	816	33.384	0.908	79.674	1.00	23.19
	1077	CB	GLU	A	816	32.522	-1.517	81.634	1.00	27.58
	1078	CG	GLU	A	816	31.621	-2.014	82.759	1.00	32.90
10	1079	CD	GLU	A	816	30.595	-3.052	82.308	1.00	38.95
	1080	OE1	GLU	A	816	30.910	-3.887	81.435	1.00	36.30
	1081	OE2	GLU	A	816	29.475	-3.052	82.861	1.00	49.03
15	1082	N	GLU	A	817	33.307	-1.066	78.606	1.00	21.48
	1083	CA	GLU	A	817	34.301	-0.666	77.613	1.00	20.83
	1084	C	GLU	A	817	33.701	0.360	76.660	1.00	20.85
20	1085	O	GLU	A	817	34.348	1.329	76.299	1.00	23.00
	1086	CB	GLU	A	817	34.778	-1.867	76.791	1.00	22.67
	1087	CG	GLU	A	817	35.660	-2.868	77.560	1.00	25.39
25	1088	CD	GLU	A	817	35.826	-4.193	76.820	1.00	33.69
	1089	OE1	GLU	A	817	34.971	-4.524	75.961	1.00	30.03
	1090	OE2	GLU	A	817	36.801	-4.917	77.103	1.00	30.51
30	1091	N	PHE	A	818	32.469	0.119	76.224	1.00	21.31
	1092	CA	PHE	A	818	31.805	1.043	75.304	1.00	22.08
	1093	C	PHE	A	818	31.696	2.467	75.884	1.00	21.29
35	1094	O	PHE	A	818	31.920	3.460	75.180	1.00	20.03
	1095	CB	PHE	A	818	30.406	0.528	75.002	1.00	23.06
	1096	CG	PHE	A	818	29.513	1.549	74.373	1.00	22.01
40	1097	CD1	PHE	A	818	29.678	1.914	73.040	1.00	22.32
	1098	CD2	PHE	A	818	28.514	2.156	75.124	1.00	23.62
	1099	CE1	PHE	A	818	28.852	2.869	72.467	1.00	27.65
45	1100	CE2	PHE	A	818	27.681	3.116	74.558	1.00	28.88
	1101	CZ	PHE	A	818	27.852	3.471	73.231	1.00	22.16
	1102	N	LEU	A	819	31.323	2.556	77.154	1.00	21.31
50	1103	CA	LEU	A	819	31.164	3.857	77.812	1.00	23.49
	1104	C	LEU	A	819	32.445	4.699	77.808	1.00	26.91
	1105	O	LEU	A	819	32.394	5.907	77.557	1.00	20.81
55	1106	CB	LEU	A	819	30.640	3.655	79.238	1.00	24.50
	1107	CG	LEU	A	819	29.199	3.116	79.294	1.00	23.57
	1108	CD1	LEU	A	819	28.780	2.812	80.728	1.00	22.54
55	1109	CD2	LEU	A	819	28.256	4.174	78.693	1.00	27.51
	1110	N	CYS	A	820	33.586	4.068	78.087	1.00	22.87
	1111	CA	CYS	A	820	34.870	4.761	78.087	1.00	26.80
	1112	C	CYS	A	820	35.306	5.082	76.656	1.00	25.96

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1113	O	CYS	A	820	35.858	6.149	76.379	1.00	20.10
	1114	CB	CYS	A	820	35.940	3.895	78.748	1.00	27.46
	1115	SG	CYS	A	820	35.550	3.486	80.454	1.00	33.20
10	1116	N	MET	A	821	35.079	4.151	75.739	1.00	18.27
	1117	CA	MET	A	821	35.456	4.420	74.371	1.00	20.73
	1118	C	MET	A	821	34.661	5.603	73.811	1.00	18.21
15	1119	O	MET	A	821	35.186	6.383	73.031	1.00	20.04
	1120	CB	MET	A	821	35.238	3.178	73.520	1.00	23.28
	1121	CG	MET	A	821	36.100	2.003	73.934	1.00	26.12
20	1122	SD	MET	A	821	35.578	0.506	73.031	1.00	30.71
	1123	CE	MET	A	821	36.127	0.928	71.492	1.00	17.04
	1124	N	LYS	A	822	33.403	5.748	74.210	1.00	22.26
25	1125	CA	LYS	A	822	32.595	6.856	73.684	1.00	21.99
	1126	C	LYS	A	822	33.157	8.208	74.120	1.00	23.71
	1127	O	LYS	A	822	33.125	9.182	73.359	1.00	20.06
30	1128	CB	LYS	A	822	31.123	6.713	74.115	1.00	24.02
	1129	CG	LYS	A	822	30.164	7.608	73.337	1.00	31.07
	1130	CD	LYS	A	822	28.727	7.077	73.410	1.00	38.28
35	1131	CE	LYS	A	822	28.155	7.091	74.822	1.00	39.48
	1132	NZ	LYS	A	822	27.958	8.479	75.331	1.00	42.42
	1133	N	VAL	A	823	33.686	8.269	75.339	1.00	20.18
40	1134	CA	VAL	A	823	34.272	9.515	75.815	1.00	19.22
	1135	C	VAL	A	823	35.541	9.802	75.028	1.00	21.84
	1136	O	VAL	A	823	35.806	10.939	74.644	1.00	21.05
45	1137	CB	VAL	A	823	34.643	9.439	77.304	1.00	19.35
	1138	CG1	VAL	A	823	35.288	10.747	77.725	1.00	18.41
	1139	CG2	VAL	A	823	33.400	9.182	78.141	1.00	23.25
50	1140	N	LEU	A	824	36.333	8.766	74.780	1.00	19.81
	1141	CA	LEU	A	824	37.561	8.950	74.019	1.00	20.73
	1142	C	LEU	A	824	37.252	9.452	72.614	1.00	24.51
55	1143	O	LEU	A	824	38.054	10.173	72.021	1.00	21.96
	1144	CB	LEU	A	824	38.371	7.644	73.976	1.00	21.13
	1145	CG	LEU	A	824	38.943	7.289	75.355	1.00	20.69
	1146	CD1	LEU	A	824	39.580	5.921	75.310	1.00	23.72
	1147	CD2	LEU	A	824	39.978	8.354	75.784	1.00	21.59
	1148	N	LEU	A	825	36.087	9.098	72.080	1.00	22.43
	1149	CA	LEU	A	825	35.712	9.582	70.758	1.00	24.57

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1150	C	LEU	A	825	35.421	11.068	70.793	1.00	22.02
1151	O	LEU	A	825	35.737	11.773	69.845	1.00	23.56
1152	CB	LEU	A	825	34.480	8.868	70.206	1.00	19.15
1153	CG	LEU	A	825	34.643	7.542	69.500	1.00	31.93
1154	CD1	LEU	A	825	33.284	7.197	68.894	1.00	28.38
1155	CD2	LEU	A	825	35.718	7.644	68.395	1.00	26.52
1156	N	LEU	A	826	34.802	11.529	71.875	1.00	18.07
1157	CA	LEU	A	826	34.507	12.948	72.046	1.00	20.16
1158	C	LEU	A	826	35.819	13.741	72.040	1.00	23.85
1159	O	LEU	A	826	35.886	14.882	71.572	1.00	23.95
1160	CB	LEU	A	826	33.805	13.171	73.384	1.00	21.07
1161	CG	LEU	A	826	33.603	14.620	73.851	1.00	22.15
1162	CD1	LEU	A	826	32.731	15.381	72.850	1.00	21.62
1163	CD2	LEU	A	826	32.966	14.629	75.234	1.00	22.53
1164	N	LEU	A	827	36.863	13.114	72.565	1.00	16.99
1165	CA	LEU	A	827	38.168	13.734	72.693	1.00	21.87
1166	C	LEU	A	827	39.134	13.226	71.637	1.00	24.10
1167	O	LEU	A	827	40.340	13.255	71.860	1.00	24.64
1168	CB	LEU	A	827	38.737	13.389	74.081	1.00	20.22
1169	CG	LEU	A	827	37.804	13.622	75.273	1.00	27.92
1170	CD1	LEU	A	827	38.451	13.115	76.571	1.00	24.44
1171	CD2	LEU	A	827	37.471	15.111	75.381	1.00	21.00
1172	N	ASN	A	828	38.638	12.797	70.477	1.00	21.55
1173	CA	ASN	A	828	39.547	12.205	69.492	1.00	26.34
1174	C	ASN	A	828	40.068	13.073	68.343	1.00	21.48
1175	O	ASN	A	828	40.831	12.604	67.501	1.00	25.22
1176	CB	ASN	A	828	38.896	10.940	68.938	1.00	24.75
1177	CG	ASN	A	828	39.862	9.775	68.868	1.00	39.47
1178	OD1	ASN	A	828	40.751	9.655	69.711	1.00	33.27
1179	ND2	ASN	A	828	39.676	8.891	67.881	1.00	37.42
1180	N	THR	A	829	39.675	14.336	68.330	1.00	20.94
1181	CA	THR	A	829	40.088	15.263	67.283	1.00	23.18
1182	C	THR	A	829	40.174	16.653	67.881	1.00	24.51
1183	O	THR	A	829	39.279	17.062	68.623	1.00	20.61
1184	CB	THR	A	829	39.047	15.287	66.125	1.00	27.14
1185	OG1	THR	A	829	38.876	13.963	65.609	1.00	27.76
1186	CG2	THR	A	829	39.512	16.196	64.987	1.00	27.52

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1187	N	ILE	A	830	41.255	17.368	67.578	1.00	23.20
	1188	CA	ILE	A	830	41.416	18.736	68.072	1.00	22.29
	1189	C	ILE	A	830	41.876	19.651	66.939	1.00	23.93
10	1190	O	ILE	A	830	42.271	19.176	65.874	1.00	23.93
	1191	CB	ILE	A	830	42.428	18.799	69.226	1.00	24.86
	1192	CG1	ILE	A	830	43.805	18.332	68.744	1.00	22.58
15	1193	CG2	ILE	A	830	41.914	17.962	70.402	1.00	25.47
	1194	CD1	ILE	A	830	44.856	18.368	69.827	1.00	28.86
	1195	N	PRO	A	831	41.818	20.971	67.150	1.00	23.63
20	1196	CA	PRO	A	831	42.240	21.919	66.117	1.00	26.05
	1197	C	PRO	A	831	43.727	21.796	65.831	1.00	30.91
	1198	O	PRO	A	831	44.496	21.316	66.673	1.00	27.25
25	1199	CB	PRO	A	831	41.888	23.277	66.732	1.00	28.62
	1200	CG	PRO	A	831	40.752	22.925	67.707	1.00	25.78
	1201	CD	PRO	A	831	41.368	21.704	68.341	1.00	28.72
30	1202	N	LEU	A	832	44.126	22.225	64.636	1.00	31.80
	1203	CA	LEU	A	832	45.528	22.180	64.238	1.00	34.58
	1204	C	LEU	A	832	46.404	22.954	65.216	1.00	32.37
35	1205	O	LEU	A	832	47.558	22.591	65.444	1.00	38.50
	1206	CB	LEU	A	832	45.699	22.760	62.827	1.00	34.68
	1207	CG	LEU	A	832	45.108	21.920	61.691	1.00	34.02
40	1208	CD1	LEU	A	832	45.298	22.624	60.342	1.00	34.39
	1209	CD2	LEU	A	832	45.787	20.563	61.686	1.00	36.07
	1210	N	GLU	A	833	45.853	24.012	65.798	1.00	33.46
45	1211	CA	GLU	A	833	46.605	24.817	66.751	1.00	35.43
	1212	C	GLU	A	833	46.379	24.348	68.188	1.00	37.02
	1213	O	GLU	A	833	46.866	24.959	69.143	1.00	34.87
50	1214	CB	GLU	A	833	46.239	26.304	66.611	1.00	40.38
	1215	CG	GLU	A	833	44.786	26.683	66.901	1.00	46.00
	1216	CD	GLU	A	833	43.802	26.239	65.825	1.00	52.16
55	1217	OE1	GLU	A	833	44.211	25.549	64.867	1.00	49.08
	1218	OE2	GLU	A	833	42.607	26.589	65.943	1.00	50.96
	1219	N	GLY	A	834	45.650	23.249	68.344	1.00	32.49
55	1220	CA	GLY	A	834	45.392	22.741	69.675	1.00	28.49
	1221	C	GLY	A	834	44.231	23.479	70.312	1.00	30.77
	1222	O	GLY	A	834	43.649	24.372	69.705	1.00	29.05
	1223	N	LEU	A	835	43.908	23.102	71.544	1.00	27.80

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1224	CA	LEU	A	835	42.812	23.691	72.297	1.00	31.88
1225	C	LEU	A	835	43.325	24.754	73.267	1.00	30.49
1226	O	LEU	A	835	44.491	24.737	73.647	1.00	28.71
1227	CB	LEU	A	835	42.119	22.595	73.102	1.00	28.43
1228	CG	LEU	A	835	41.438	21.461	72.335	1.00	31.10
1229	CD1	LEU	A	835	41.071	20.363	73.310	1.00	29.92
1230	CD2	LEU	A	835	40.200	21.995	71.598	1.00	27.76
1231	N	ARG	A	836	42.446	25.659	73.685	1.00	33.09
1232	CA	ARG	A	836	42.839	26.695	74.644	1.00	33.34
1233	C	ARG	A	836	43.209	26.019	75.973	1.00	37.41
1234	O	ARG	A	836	44.155	26.427	76.662	1.00	35.58
1235	CB	ARG	A	836	41.683	27.673	74.872	1.00	37.62
1236	CG	ARG	A	836	41.129	28.268	73.591	1.00	43.12
1237	CD	ARG	A	836	40.175	29.438	73.840	1.00	55.06
1238	NE	ARG	A	836	40.858	30.690	74.181	1.00	65.30
1239	CZ	ARG	A	836	41.461	30.952	75.339	1.00	65.60
1240	NH1	ARG	A	836	41.467	30.059	76.319	1.00	69.19
1241	NH2	ARG	A	836	42.048	32.127	75.525	1.00	71.09
1242	N	SER	A	837	42.439	24.994	76.337	1.00	28.39
1243	CA	SER	A	837	42.672	24.234	77.557	1.00	29.00
1244	C	SER	A	837	43.364	22.924	77.192	1.00	30.23
1245	O	SER	A	837	42.910	21.851	77.576	1.00	26.81
1246	CB	SER	A	837	41.339	23.933	78.249	1.00	23.84
1247	OG	SER	A	837	40.660	25.131	78.575	1.00	31.90
1248	N	GLN	A	838	44.467	23.007	76.452	1.00	29.41
1249	CA	GLN	A	838	45.162	21.796	76.031	1.00	28.12
1250	C	GLN	A	838	45.642	20.947	77.207	1.00	30.39
1251	O	GLN	A	838	45.503	19.730	77.190	1.00	26.03
1252	CB	GLN	A	838	46.341	22.154	75.125	1.00	25.64
1253	CG	GLN	A	838	46.954	20.986	74.371	1.00	32.23
1254	CD	GLN	A	838	45.976	20.338	73.401	1.00	37.10
1255	OE1	GLN	A	838	45.199	21.021	72.730	1.00	37.64
1256	NE2	GLN	A	838	46.028	19.017	73.306	1.00	42.95
1257	N	THR	A	839	46.224	21.578	78.224	1.00	27.88
1258	CA	THR	A	839	46.688	20.825	79.385	1.00	30.26
1259	C	THR	A	839	45.573	20.042	80.054	1.00	27.76
1260	O	THR	A	839	45.724	18.847	80.322	1.00	28.54

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1261	CB	THR	A	839	47.298	21.744	80.436	1.00	31.84
	1262	OG1	THR	A	839	48.408	22.426	79.857	1.00	38.66
	1263	CG2	THR	A	839	47.766	20.939	81.643	1.00	35.08
10	1264	N	GLN	A	840	44.466	20.725	80.337	1.00	27.40
	1265	CA	GLN	A	840	43.314	20.095	80.964	1.00	27.76
	1266	C	GLN	A	840	42.790	18.986	80.059	1.00	27.08
15	1267	O	GLN	A	840	42.382	17.926	80.534	1.00	24.43
	1268	CB	GLN	A	840	42.199	21.106	81.205	1.00	29.57
	1269	CG	GLN	A	840	42.471	22.127	82.286	1.00	46.45
20	1270	CD	GLN	A	840	41.237	22.957	82.640	1.00	53.97
	1271	OE1	GLN	A	840	40.747	23.754	81.829	1.00	56.14
	1272	NE2	GLN	A	840	40.723	22.763	83.852	1.00	51.09
25	1273	N	PHE	A	841	42.821	19.235	78.757	1.00	25.08
	1274	CA	PHE	A	841	42.343	18.247	77.788	1.00	25.20
	1275	C	PHE	A	841	43.192	16.985	77.814	1.00	22.17
30	1276	O	PHE	A	841	42.661	15.871	77.804	1.00	24.69
	1277	CB	PHE	A	841	42.312	18.858	76.381	1.00	24.39
	1278	CG	PHE	A	841	42.136	17.846	75.275	1.00	25.18
35	1279	CD1	PHE	A	841	40.857	17.414	74.898	1.00	26.95
	1280	CD2	PHE	A	841	43.243	17.288	74.642	1.00	21.90
	1281	CE1	PHE	A	841	40.690	16.435	73.898	1.00	22.61
40	1282	CE2	PHE	A	841	43.092	16.309	73.645	1.00	21.56
	1283	CZ	PHE	A	841	41.813	15.880	73.274	1.00	23.75
	1284	N	GLU	A	842	44.506	17.155	77.855	1.00	26.80
45	1285	CA	GLU	A	842	45.423	16.012	77.905	1.00	30.80
	1286	C	GLU	A	842	45.156	15.160	79.144	1.00	27.28
	1287	O	GLU	A	842	45.093	13.933	79.073	1.00	27.77
50	1288	CB	GLU	A	842	46.879	16.489	77.963	1.00	28.70
	1289	CG	GLU	A	842	47.746	15.961	76.851	1.00	50.83
	1290	CD	GLU	A	842	47.567	16.720	75.552	1.00	54.53
55	1291	OE1	GLU	A	842	48.053	17.872	75.456	1.00	61.42
	1292	OE2	GLU	A	842	46.940	16.166	74.626	1.00	61.75
	1293	N	GLU	A	843	45.039	15.820	80.289	1.00	29.50
55	1294	CA	GLU	A	843	44.776	15.123	81.539	1.00	27.52
	1295	C	GLU	A	843	43.439	14.385	81.472	1.00	29.29
	1296	O	GLU	A	843	43.311	13.263	81.942	1.00	29.26
	1297	CB	GLU	A	843	44.767	16.110	82.713	1.00	32.59

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1298	CG	GLU	A	843	46.149	16.594	83.160	1.00	38.26
1299	CD	GLU	A	843	46.080	17.675	84.235	1.00	47.34
1300	OE1	GLU	A	843	45.229	17.570	85.144	1.00	51.54
1301	OE2	GLU	A	843	46.893	18.625	84.187	1.00	49.88
1302	N	MET	A	844	42.439	15.015	80.878	1.00	25.95
1303	CA	MET	A	844	41.141	14.377	80.788	1.00	26.70
1304	C	MET	A	844	41.233	13.125	79.929	1.00	26.41
1305	O	MET	A	844	40.770	12.050	80.314	1.00	25.61
1306	CB	MET	A	844	40.128	15.351	80.203	1.00	26.67
1307	CG	MET	A	844	38.737	14.761	80.116	1.00	30.25
1308	SD	MET	A	844	37.486	15.952	79.605	1.00	28.34
1309	CE	MET	A	844	36.074	14.840	79.459	1.00	23.92
1310	N	ARG	A	845	41.860	13.264	78.769	1.00	26.84
1311	CA	ARG	A	845	42.001	12.140	77.864	1.00	29.65
1312	C	ARG	A	845	42.753	10.981	78.546	1.00	31.46
1313	O	ARG	A	845	42.335	9.831	78.466	1.00	28.49
1314	CB	ARG	A	845	42.700	12.616	76.590	1.00	29.38
1315	CG	ARG	A	845	42.609	11.649	75.433	1.00	38.40
1316	CD	ARG	A	845	43.039	12.303	74.132	1.00	33.58
1317	NE	ARG	A	845	42.924	11.361	73.022	1.00	43.23
1318	CZ	ARG	A	845	43.763	10.357	72.807	1.00	45.03
1319	NH1	ARG	A	845	44.806	10.180	73.610	1.00	58.21
1320	NH2	ARG	A	845	43.578	9.545	71.772	1.00	52.78
1321	N	SER	A	846	43.844	11.284	79.241	1.00	29.00
1322	CA	SER	A	846	44.605	10.243	79.935	1.00	29.23
1323	C	SER	A	846	43.777	9.537	81.004	1.00	25.05
1324	O	SER	A	846	43.882	8.328	81.179	1.00	27.74
1325	CB	SER	A	846	45.863	10.840	80.567	1.00	29.17
1326	OG	SER	A	846	46.745	11.267	79.550	1.00	35.25
1327	N	SER	A	847	42.966	10.298	81.727	1.00	27.46
1328	CA	SER	A	847	42.116	9.736	82.769	1.00	26.94
1329	C	SER	A	847	41.134	8.736	82.170	1.00	28.69
1330	O	SER	A	847	40.870	7.692	82.753	1.00	24.01
1331	CB	SER	A	847	41.346	10.849	83.482	1.00	33.23
1332	OG	SER	A	847	42.249	11.709	84.158	1.00	39.50
1333	N	TYR	A	848	40.587	9.056	81.005	1.00	23.69
1334	CA	TYR	A	848	39.648	8.141	80.369	1.00	24.43

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1335	C	TYR	A	848	40.336	6.957	79.707	1.00	25.10
	1336	O	TYR	A	848	39.747	5.888	79.586	1.00	24.91
	1337	CB	TYR	A	848	38.762	8.913	79.402	1.00	22.98
10	1338	CG	TYR	A	848	37.683	9.651	80.152	1.00	21.21
	1339	CD1	TYR	A	848	36.543	8.975	80.595	1.00	21.26
	1340	CD2	TYR	A	848	37.816	11.003	80.459	1.00	21.12
15	1341	CE1	TYR	A	848	35.551	9.624	81.324	1.00	22.44
	1342	CE2	TYR	A	848	36.828	11.665	81.191	1.00	23.86
	1343	CZ	TYR	A	848	35.693	10.968	81.619	1.00	28.65
20	1344	OH	TYR	A	848	34.686	11.611	82.319	1.00	23.47
	1345	N	ILE	A	849	41.581	7.133	79.289	1.00	23.21
	1346	CA	ILE	A	849	42.314	6.019	78.714	1.00	29.14
25	1347	C	ILE	A	849	42.566	5.060	79.879	1.00	30.21
	1348	O	ILE	A	849	42.446	3.846	79.744	1.00	26.87
	1349	CB	ILE	A	849	43.654	6.488	78.069	1.00	29.35
30	1350	CG1	ILE	A	849	43.356	7.281	76.790	1.00	23.92
	1351	CG2	ILE	A	849	44.547	5.291	77.729	1.00	27.00
	1352	CD1	ILE	A	849	44.583	7.816	76.109	1.00	22.76
35	1353	N	ARG	A	850	42.889	5.608	81.043	1.00	28.71
	1354	CA	ARG	A	850	43.113	4.753	82.195	1.00	32.10
	1355	C	ARG	A	850	41.816	4.078	82.611	1.00	29.94
40	1356	O	ARG	A	850	41.824	2.959	83.107	1.00	28.11
	1357	CB	ARG	A	850	43.672	5.538	83.387	1.00	35.86
	1358	CG	ARG	A	850	45.100	6.028	83.221	1.00	40.68
45	1359	CD	ARG	A	850	45.662	6.509	84.558	1.00	46.12
	1360	NE	ARG	A	850	44.999	7.702	85.079	1.00	48.88
	1361	CZ	ARG	A	850	45.160	8.924	84.581	1.00	47.54
50	1362	NH1	ARG	A	850	45.964	9.121	83.546	1.00	47.38
	1363	NH2	ARG	A	850	44.515	9.952	85.115	1.00	52.75
	1364	N	GLU	A	851	40.691	4.750	82.408	1.00	26.26
55	1365	CA	GLU	A	851	39.428	4.149	82.798	1.00	24.07
	1366	C	GLU	A	851	39.058	3.010	81.843	1.00	25.19
	1367	O	GLU	A	851	38.480	2.005	82.269	1.00	27.72
	1368	CB	GLU	A	851	38.325	5.209	82.851	1.00	29.75
	1369	CG	GLU	A	851	37.158	4.816	83.735	1.00	32.34
	1370	CD	GLU	A	851	37.559	4.663	85.207	1.00	48.72
	1371	OE1	GLU	A	851	38.709	5.013	85.558	1.00	47.00

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1372	OE2	GLU	A	851	36.723	4.202	86.018	1.00	46.97
1373	N	LEU	A	852	39.390	3.158	80.562	1.00	23.97
1374	CA	LEU	A	852	39.127	2.104	79.584	1.00	22.66
1375	C	LEU	A	852	39.945	0.872	79.992	1.00	30.81
1376	O	LEU	A	852	39.490	-0.260	79.844	1.00	24.16
1377	CB	LEU	A	852	39.572	2.547	78.186	1.00	22.80
1378	CG	LEU	A	852	39.595	1.452	77.115	1.00	25.24
1379	CD1	LEU	A	852	38.196	0.939	76.908	1.00	25.51
1380	CD2	LEU	A	852	40.186	1.996	75.801	1.00	27.39
1381	N	ILE	A	853	41.167	1.096	80.474	1.00	24.04
1382	CA	ILE	A	853	42.008	-0.021	80.897	1.00	29.31
1383	C	ILE	A	853	41.328	-0.764	82.035	1.00	28.39
1384	O	ILE	A	853	41.275	-1.994	82.025	1.00	28.22
1385	CB	ILE	A	853	43.418	0.461	81.316	1.00	32.13
1386	CG1	ILE	A	853	44.150	0.976	80.077	1.00	26.53
1387	CG2	ILE	A	853	44.212	-0.686	81.980	1.00	26.27
1388	CD1	ILE	A	853	45.496	1.620	80.364	1.00	29.29
1389	N	LYS	A	854	40.778	-0.025	82.999	1.00	29.91
1390	CA	LYS	A	854	40.070	-0.645	84.121	1.00	27.78
1391	C	LYS	A	854	38.861	-1.428	83.616	1.00	28.75
1392	O	LYS	A	854	38.564	-2.515	84.106	1.00	30.96
1393	CB	LYS	A	854	39.594	0.408	85.121	1.00	32.36
1394	CG	LYS	A	854	40.695	1.151	85.839	1.00	32.65
1395	CD	LYS	A	854	40.084	2.199	86.763	1.00	41.08
1396	CE	LYS	A	854	41.158	3.004	87.445	1.00	47.72
1397	NZ	LYS	A	854	42.079	3.620	86.445	1.00	54.97
1398	N	ALA	A	855	38.154	-0.875	82.634	1.00	25.66
1399	CA	ALA	A	855	36.981	-1.561	82.099	1.00	26.89
1400	C	ALA	A	855	37.422	-2.887	81.490	1.00	25.18
1401	O	ALA	A	855	36.761	-3.914	81.667	1.00	24.74
1402	CB	ALA	A	855	36.292	-0.698	81.038	1.00	22.45
1403	N	ILE	A	856	38.543	-2.853	80.780	1.00	25.69
1404	CA	ILE	A	856	39.079	-4.051	80.132	1.00	28.42
1405	C	ILE	A	856	39.473	-5.061	81.212	1.00	32.00
1406	O	ILE	A	856	39.232	-6.258	81.066	1.00	33.59
1407	CB	ILE	A	856	40.297	-3.690	79.258	1.00	31.03
1408	CG1	ILE	A	856	39.817	-2.913	78.024	1.00	25.53

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1409	CG2	ILE	A	856	41.066	-4.950	78.854	1.00	29.18
	1410	CD1	ILE	A	856	40.940	-2.382	77.164	1.00	27.39
	1411	N	GLY	A	857	40.060	-4.559	82.294	1.00	33.82
10	1412	CA	GLY	A	857	40.475	-5.410	83.397	1.00	34.58
	1413	C	GLY	A	857	39.345	-6.137	84.105	1.00	37.55
	1414	O	GLY	A	857	39.566	-7.165	84.749	1.00	37.64
15	1415	N	LEU	A	858	38.129	-5.615	83.994	1.00	33.59
	1416	CA	LEU	A	858	36.981	-6.237	84.630	1.00	37.87
	1417	C	LEU	A	858	36.730	-7.652	84.110	1.00	42.05
20	1418	O	LEU	A	858	36.162	-8.482	84.816	1.00	37.32
	1419	CB	LEU	A	858	35.723	-5.393	84.404	1.00	35.77
	1420	CG	LEU	A	858	35.707	-3.981	84.980	1.00	34.70
25	1421	CD1	LEU	A	858	34.393	-3.311	84.614	1.00	39.67
	1422	CD2	LEU	A	858	35.873	-4.036	86.488	1.00	40.03
	1423	N	ARG	A	859	37.161	-7.921	82.880	1.00	42.57
30	1424	CA	ARG	A	859	36.947	-9.221	82.256	1.00	52.08
	1425	C	ARG	A	859	38.188	-9.797	81.586	1.00	54.79
	1426	O	ARG	A	859	38.201	-10.972	81.215	1.00	58.54
35	1427	CB	ARG	A	859	35.820	-9.121	81.226	1.00	52.12
	1428	CG	ARG	A	859	34.472	-8.758	81.830	1.00	58.32
	1429	CD	ARG	A	859	33.381	-8.622	80.776	1.00	61.04
40	1430	NE	ARG	A	859	32.082	-8.385	81.399	1.00	72.95
	1431	CZ	ARG	A	859	30.938	-8.230	80.737	1.00	76.45
	1432	NH1	ARG	A	859	30.918	-8.279	79.411	1.00	80.87
45	1433	NH2	ARG	A	859	29.810	-8.021	81.406	1.00	77.97
	1434	N	GLN	A	860	39.222	-8.976	81.416	1.00	60.36
	1435	CA	GLN	A	860	40.460	-9.442	80.800	1.00	65.05
50	1436	C	GLN	A	860	41.558	-9.610	81.840	1.00	67.98
	1437	O	GLN	A	860	42.356	-8.704	82.096	1.00	68.79
	1438	CB	GLN	A	860	40.910	-8.493	79.688	1.00	64.71
55	1439	CG	GLN	A	860	39.943	-8.453	78.519	1.00	68.26
	1440	CD	GLN	A	860	39.754	-9.810	77.861	1.00	71.18
	1441	OE1	GLN	A	860	38.897	-9.980	76.991	1.00	72.78
60	1442	NE2	GLN	A	860	40.561	-10.784	78.268	1.00	72.46
	1443	N	LYS	A	861	41.560	-10.798	82.434	1.00	70.37
	1444	CA	LYS	A	861	42.507	-11.206	83.459	1.00	71.87
65	1445	C	LYS	A	861	43.962	-11.197	82.978	1.00	72.34

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	1446	O	LYS	A	861	44.825	-10.575	83.603	1.00	71.39
	1447	CB	LYS	A	861	42.111	-12.604	83.946	1.00	74.09
	1448	CG	LYS	A	861	41.860	-13.587	82.797	1.00	76.68
10	1449	CD	LYS	A	861	41.293	-14.925	83.273	1.00	77.75
	1450	CE	LYS	A	861	40.977	-15.836	82.086	1.00	77.67
	1451	NZ	LYS	A	861	40.368	-17.136	82.492	1.00	78.97
15	1452	N	GLY	A	862	44.230	-11.885	81.870	1.00	72.03
	1453	CA	GLY	A	862	45.583	-11.943	81.340	1.00	72.71
	1454	C	GLY	A	862	46.226	-10.580	81.144	1.00	71.15
20	1455	O	GLY	A	862	45.589	-9.655	80.644	1.00	71.21
	1456	N	VAL	A	863	47.489	-10.452	81.535	1.00	70.79
	1457	CA	VAL	A	863	48.212	-9.191	81.392	1.00	69.40
25	1458	C	VAL	A	863	48.467	-8.888	79.918	1.00	68.93
	1459	O	VAL	A	863	48.543	-7.723	79.516	1.00	66.12
	1460	CB	VAL	A	863	49.574	-9.234	82.125	1.00	71.43
30	1461	CG1	VAL	A	863	49.359	-9.445	83.617	1.00	70.39
	1462	CG2	VAL	A	863	50.441	-10.347	81.544	1.00	72.36
	1463	N	VAL	A	864	48.605	-9.943	79.120	1.00	65.17
35	1464	CA	VAL	A	864	48.848	-9.782	77.693	1.00	64.59
	1465	C	VAL	A	864	47.511	-9.789	76.963	1.00	61.44
	1466	O	VAL	A	864	47.331	-9.088	75.971	1.00	61.24
40	1467	CB	VAL	A	864	49.744	-10.916	77.139	1.00	65.52
	1468	CG1	VAL	A	864	49.034	-12.258	77.263	1.00	67.34
	1469	CG2	VAL	A	864	50.117	-10.624	75.691	1.00	65.68
45	1470	N	SER	A	865	46.574	-10.588	77.464	1.00	58.29
	1471	CA	SER	A	865	45.250	-10.666	76.868	1.00	52.84
	1472	C	SER	A	865	44.584	-9.299	77.017	1.00	51.66
50	1473	O	SER	A	865	43.901	-8.825	76.109	1.00	45.86
	1474	CB	SER	A	865	44.410	-11.733	77.572	1.00	55.37
	1475	OG	SER	A	865	43.096	-11.778	77.043	1.00	56.88
55	1476	N	SER	A	866	44.798	-8.674	78.169	1.00	44.60
	1477	CA	SER	A	866	44.234	-7.361	78.442	1.00	45.64
	1478	C	SER	A	866	44.961	-6.340	77.581	1.00	44.47
55	1479	O	SER	A	866	44.375	-5.360	77.123	1.00	39.29
	1480	CB	SER	A	866	44.417	-6.997	79.914	1.00	45.32
	1481	OG	SER	A	866	45.788	-6.829	80.218	1.00	48.12
	1482	N	SER	A	867	46.247	-6.587	77.367	1.00	43.23

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1483	CA	SER	A	867	47.077	-5.707	76.565	1.00	42.20
	1484	C	SER	A	867	46.642	-5.804	75.109	1.00	41.29
	1485	O	SER	A	867	46.510	-4.791	74.420	1.00	42.13
10	1486	CB	SER	A	867	48.547	-6.107	76.706	1.00	43.71
	1487	OG	SER	A	867	49.383	-5.173	76.055	1.00	50.34
	1488	N	GLN	A	868	46.420	-7.028	74.640	1.00	35.72
15	1489	CA	GLN	A	868	45.982	-7.234	73.270	1.00	36.75
	1490	C	GLN	A	868	44.575	-6.663	73.101	1.00	31.61
	1491	O	GLN	A	868	44.198	-6.218	72.017	1.00	34.73
20	1492	CB	GLN	A	868	46.006	-8.727	72.927	1.00	41.06
	1493	CG	GLN	A	868	47.410	-9.332	73.045	1.00	51.40
	1494	CD	GLN	A	868	47.458	-10.819	72.756	1.00	56.24
25	1495	OE1	GLN	A	868	47.151	-11.263	71.647	1.00	66.21
	1496	NE2	GLN	A	868	47.850	-11.603	73.756	1.00	61.83
	1497	N	ARG	A	869	43.815	-6.667	74.188	1.00	30.91
30	1498	CA	ARG	A	869	42.443	-6.153	74.193	1.00	33.76
	1499	C	ARG	A	869	42.483	-4.639	74.028	1.00	29.74
	1500	O	ARG	A	869	41.703	-4.053	73.274	1.00	28.46
35	1501	CB	ARG	A	869	41.781	-6.493	75.521	1.00	31.23
	1502	CG	ARG	A	869	40.335	-6.051	75.662	1.00	40.84
	1503	CD	ARG	A	869	39.462	-6.760	74.664	1.00	36.78
40	1504	NE	ARG	A	869	38.039	-6.531	74.910	1.00	41.13
	1505	CZ	ARG	A	869	37.079	-7.104	74.198	1.00	35.24
	1506	NH1	ARG	A	869	37.410	-7.936	73.217	1.00	32.73
45	1507	NH2	ARG	A	869	35.805	-6.857	74.464	1.00	33.12
	1508	N	PHE	A	870	43.405	-4.017	74.748	1.00	27.87
	1509	CA	PHE	A	870	43.561	-2.578	74.691	1.00	29.28
50	1510	C	PHE	A	870	43.929	-2.212	73.268	1.00	30.03
	1511	O	PHE	A	870	43.410	-1.244	72.707	1.00	29.75
	1512	CB	PHE	A	870	44.655	-2.123	75.644	1.00	30.24
55	1513	CG	PHE	A	870	44.801	-0.631	75.724	1.00	32.22
	1514	CD1	PHE	A	870	43.875	0.136	76.426	1.00	30.59
	1515	CD2	PHE	A	870	45.859	0.008	75.089	1.00	33.43
55	1516	CE1	PHE	A	870	44.004	1.522	76.496	1.00	29.82
	1517	CE2	PHE	A	870	45.996	1.389	75.152	1.00	33.14
	1518	CZ	PHE	A	870	45.064	2.149	75.859	1.00	28.67
	1519	N	TYR	A	871	44.805	-3.010	72.667	1.00	28.46

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1520	CA	TYR	A	871	45.230	-2.753	71.297	1.00	33.75
1521	C	TYR	A	871	44.060	-2.815	70.326	1.00	30.34
1522	O	TYR	A	871	43.918	-1.949	69.466	1.00	31.44
1523	CB	TYR	A	871	46.286	-3.765	70.835	1.00	32.68
1524	CG	TYR	A	871	46.685	-3.571	69.387	1.00	39.92
1525	CD1	TYR	A	871	47.512	-2.519	69.003	1.00	45.08
1526	CD2	TYR	A	871	46.182	-4.404	68.390	1.00	45.67
1527	CE1	TYR	A	871	47.829	-2.297	67.656	1.00	52.13
1528	CE2	TYR	A	871	46.488	-4.192	67.042	1.00	51.47
1529	CZ	TYR	A	871	47.310	-3.139	66.682	1.00	51.04
1530	OH	TYR	A	871	47.608	-2.930	65.351	1.00	54.66
1531	N	GLN	A	872	43.238	-3.849	70.465	1.00	27.62
1532	CA	GLN	A	872	42.087	-4.041	69.601	1.00	28.60
1533	C	GLN	A	872	41.069	-2.908	69.710	1.00	30.83
1534	O	GLN	A	872	40.583	-2.386	68.696	1.00	26.66
1535	CB	GLN	A	872	41.392	-5.355	69.940	1.00	34.35
1536	CG	GLN	A	872	42.276	-6.586	69.790	1.00	38.32
1537	CD	GLN	A	872	41.536	-7.857	70.141	1.00	43.83
1538	OE1	GLN	A	872	41.009	-8.001	71.246	1.00	44.13
1539	NE2	GLN	A	872	41.492	-8.788	69.204	1.00	49.31
1540	N	LEU	A	873	40.744	-2.537	70.941	1.00	26.84
1541	CA	LEU	A	873	39.768	-1.477	71.159	1.00	25.39
1542	C	LEU	A	873	40.261	-0.121	70.665	1.00	27.79
1543	O	LEU	A	873	39.494	0.632	70.052	1.00	27.31
1544	CB	LEU	A	873	39.391	-1.399	72.642	1.00	24.65
1545	CG	LEU	A	873	38.754	-2.687	73.190	1.00	26.51
1546	CD1	LEU	A	873	38.334	-2.516	74.626	1.00	29.15
1547	CD2	LEU	A	873	37.565	-3.064	72.327	1.00	24.41
1548	N	THR	A	874	41.528	0.195	70.920	1.00	26.19
1549	CA	THR	A	874	42.068	1.473	70.481	1.00	29.70
1550	C	THR	A	874	42.277	1.478	68.965	1.00	32.67
1551	O	THR	A	874	42.227	2.533	68.322	1.00	30.17
1552	CB	THR	A	874	43.385	1.837	71.234	1.00	29.72
1553	OG1	THR	A	874	44.377	0.827	71.031	1.00	33.15
1554	CG2	THR	A	874	43.117	1.965	72.715	1.00	32.70
1555	N	LYS	A	875	42.489	0.306	68.377	1.00	29.23
1556	CA	LYS	A	875	42.661	0.249	66.930	1.00	29.94

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1557	C	LYS	A	875	41.290	0.526	66.311	1.00	25.15
	1558	O	LYS	A	875	41.184	1.171	65.284	1.00	30.87
	1559	CB	LYS	A	875	43.173	-1.135	66.495	1.00	32.66
10	1560	CG	LYS	A	875	43.612	-1.210	65.033	1.00	41.23
	1561	CD	LYS	A	875	44.781	-0.267	64.756	1.00	45.10
	1562	CE	LYS	A	875	45.193	-0.300	63.295	1.00	45.88
15	1563	NZ	LYS	A	875	46.368	0.572	63.042	1.00	50.22
	1564	N	LEU	A	876	40.232	0.047	66.954	1.00	28.84
	1565	CA	LEU	A	876	38.875	0.282	66.460	1.00	30.79
20	1566	C	LEU	A	876	38.587	1.794	66.451	1.00	31.46
	1567	O	LEU	A	876	38.047	2.329	65.479	1.00	28.53
	1568	CB	LEU	A	876	37.864	-0.458	67.333	1.00	29.92
25	1569	CG	LEU	A	876	36.369	-0.362	66.999	1.00	36.08
	1570	CD1	LEU	A	876	35.623	-1.521	67.641	1.00	37.87
	1571	CD2	LEU	A	876	35.817	0.960	67.493	1.00	34.23
30	1572	N	LEU	A	877	38.960	2.481	67.525	1.00	26.83
	1573	CA	LEU	A	877	38.750	3.926	67.590	1.00	32.06
	1574	C	LEU	A	877	39.517	4.622	66.465	1.00	31.54
35	1575	O	LEU	A	877	38.984	5.538	65.816	1.00	27.43
	1576	CB	LEU	A	877	39.191	4.472	68.950	1.00	28.40
	1577	CG	LEU	A	877	38.327	4.058	70.146	1.00	33.60
40	1578	CD1	LEU	A	877	38.892	4.669	71.418	1.00	27.76
	1579	CD2	LEU	A	877	36.880	4.525	69.941	1.00	36.94
	1580	N	ASP	A	878	40.765	4.203	66.238	1.00	30.89
45	1581	CA	ASP	A	878	41.568	4.782	65.157	1.00	31.45
	1582	C	ASP	A	878	40.853	4.591	63.829	1.00	33.06
	1583	O	ASP	A	878	40.771	5.522	63.026	1.00	27.21
50	1584	CB	ASP	A	878	42.946	4.113	65.033	1.00	32.85
	1585	CG	ASP	A	878	43.925	4.541	66.118	1.00	41.09
	1586	OD1	ASP	A	878	43.584	5.414	66.944	1.00	34.77
55	1587	OD2	ASP	A	878	45.055	3.994	66.134	1.00	35.56
	1588	N	ASN	A	879	40.356	3.377	63.588	1.00	23.23
	1589	CA	ASN	A	879	39.665	3.101	62.334	1.00	29.88
55	1590	C	ASN	A	879	38.387	3.907	62.137	1.00	27.44
	1591	O	ASN	A	879	37.949	4.114	61.006	1.00	28.18
	1592	CB	ASN	A	879	39.367	1.600	62.197	1.00	30.74
	1593	CG	ASN	A	879	40.637	0.764	62.168	1.00	34.40

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1594	OD1	ASN	A	879	41.648	1.178	61.596	1.00	41.39
1595	ND2	ASN	A	879	40.584	-0.423	62.760	1.00	42.87
1596	N	LEU	A	880	37.796	4.383	63.226	1.00	27.04
1597	CA	LEU	A	880	36.576	5.177	63.100	1.00	28.38
1598	C	LEU	A	880	36.792	6.459	62.283	1.00	29.38
1599	O	LEU	A	880	35.886	6.927	61.585	1.00	26.74
1600	CB	LEU	A	880	36.018	5.508	64.484	1.00	27.75
1601	CG	LEU	A	880	35.486	4.285	65.230	1.00	38.99
1602	CD1	LEU	A	880	35.009	4.692	66.610	1.00	40.02
1603	CD2	LEU	A	880	34.350	3.650	64.436	1.00	40.28
1604	N	HIS	A	881	37.991	7.021	62.354	1.00	25.82
1605	CA	HIS	A	881	38.286	8.241	61.605	1.00	26.55
1606	C	HIS	A	881	37.990	8.104	60.114	1.00	28.01
1607	O	HIS	A	881	37.313	8.950	59.539	1.00	26.18
1608	CB	HIS	A	881	39.749	8.666	61.806	1.00	27.98
1609	CG	HIS	A	881	40.008	9.366	63.105	1.00	31.07
1610	ND1	HIS	A	881	40.931	8.916	64.026	1.00	34.25
1611	CD2	HIS	A	881	39.492	10.509	63.619	1.00	25.45
1612	CE1	HIS	A	881	40.974	9.753	65.049	1.00	30.14
1613	NE2	HIS	A	881	40.110	10.727	64.826	1.00	32.22
1614	N	ASP	A	882	38.468	7.039	59.481	1.00	30.88
1615	CA	ASP	A	882	38.218	6.873	58.049	1.00	33.37
1616	C	ASP	A	882	36.746	6.575	57.802	1.00	32.18
1617	O	ASP	A	882	36.169	7.037	56.819	1.00	28.61
1618	CB	ASP	A	882	39.082	5.750	57.472	1.00	41.89
1619	CG	ASP	A	882	39.088	5.738	55.943	1.00	53.35
1620	OD1	ASP	A	882	39.469	6.768	55.336	1.00	57.38
1621	OD2	ASP	A	882	38.721	4.697	55.346	1.00	62.05
1622	N	LEU	A	883	36.139	5.796	58.692	1.00	25.95
1623	CA	LEU	A	883	34.728	5.467	58.558	1.00	24.45
1624	C	LEU	A	883	33.864	6.732	58.623	1.00	24.31
1625	O	LEU	A	883	33.015	6.966	57.764	1.00	24.16
1626	CB	LEU	A	883	34.306	4.481	59.660	1.00	25.35
1627	CG	LEU	A	883	32.882	3.908	59.636	1.00	28.35
1628	CD1	LEU	A	883	32.814	2.745	60.621	1.00	31.42
1629	CD2	LEU	A	883	31.847	4.957	59.983	1.00	26.70
1630	N	VAL	A	884	34.081	7.539	59.655	1.00	23.01

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1631	CA	VAL	A	884	33.314	8.771	59.837	1.00	25.27
	1632	C	VAL	A	884	33.474	9.762	58.678	1.00	22.87
	1633	O	VAL	A	884	32.551	10.522	58.359	1.00	21.03
10	1634	CB	VAL	A	884	33.715	9.458	61.162	1.00	28.67
	1635	CG1	VAL	A	884	33.064	10.827	61.263	1.00	30.03
	1636	CG2	VAL	A	884	33.274	8.588	62.338	1.00	28.50
15	1637	N	LYS	A	885	34.642	9.757	58.055	1.00	23.37
	1638	CA	LYS	A	885	34.886	10.649	56.926	1.00	23.75
	1639	C	LYS	A	885	33.895	10.401	55.788	1.00	24.31
20	1640	O	LYS	A	885	33.477	11.343	55.109	1.00	23.94
	1641	CB	LYS	A	885	36.309	10.477	56.418	1.00	23.23
	1642	CG	LYS	A	885	36.681	11.476	55.335	1.00	34.73
25	1643	CD	LYS	A	885	38.164	11.383	54.997	1.00	40.32
	1644	CE	LYS	A	885	38.563	12.449	53.990	1.00	45.17
	1645	NZ	LYS	A	885	40.031	12.437	53.725	1.00	50.18
30	1646	N	GLN	A	886	33.513	9.140	55.574	1.00	20.06
	1647	CA	GLN	A	886	32.547	8.829	54.523	1.00	21.61
	1648	C	GLN	A	886	31.185	9.358	54.940	1.00	20.55
35	1649	O	GLN	A	886	30.423	9.843	54.104	1.00	21.72
	1650	CB	GLN	A	886	32.453	7.319	54.275	1.00	27.13
	1651	CG	GLN	A	886	33.795	6.688	54.059	1.00	32.13
40	1652	CD	GLN	A	886	33.718	5.402	53.291	1.00	45.67
	1653	OE1	GLN	A	886	33.018	4.467	53.680	1.00	52.55
	1654	NE2	GLN	A	886	34.453	5.337	52.185	1.00	51.53
45	1655	N	LEU	A	887	30.859	9.241	56.226	1.00	18.60
	1656	CA	LEU	A	887	29.591	9.768	56.707	1.00	19.89
	1657	C	LEU	A	887	29.602	11.309	56.577	1.00	21.61
50	1658	O	LEU	A	887	28.607	11.911	56.172	1.00	18.84
	1659	CB	LEU	A	887	29.363	9.362	58.163	1.00	24.80
	1660	CG	LEU	A	887	29.337	7.867	58.499	1.00	32.83
55	1661	CD1	LEU	A	887	28.908	7.716	59.961	1.00	30.42
	1662	CD2	LEU	A	887	28.362	7.129	57.600	1.00	34.48
	1663	N	HIS	A	888	30.722	11.949	56.922	1.00	20.58
55	1664	CA	HIS	A	888	30.834	13.416	56.812	1.00	19.88
	1665	C	HIS	A	888	30.633	13.886	55.368	1.00	23.80
	1666	O	HIS	A	888	29.931	14.867	55.107	1.00	21.80
	1667	CB	HIS	A	888	32.205	13.878	57.303	1.00	21.04

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1668	CG	HIS	A	888	32.338	13.932	58.792	1.00	19.68
1669	ND1	HIS	A	888	33.561	13.960	59.424	1.00	21.40
1670	CD2	HIS	A	888	31.407	14.036	59.768	1.00	20.80
1671	CE1	HIS	A	888	33.378	14.080	60.728	1.00	24.56
1672	NE2	HIS	A	888	32.081	14.129	60.964	1.00	26.11
1673	N	LEU	A	889	31.248	13.178	54.426	1.00	22.67
1674	CA	LEU	A	889	31.114	13.550	53.025	1.00	21.83
1675	C	LEU	A	889	29.679	13.377	52.530	1.00	21.54
1676	O	LEU	A	889	29.144	14.251	51.854	1.00	20.75
1677	CB	LEU	A	889	32.056	12.712	52.174	1.00	20.66
1678	CG	LEU	A	889	32.041	13.046	50.683	1.00	26.71
1679	CD1	LEU	A	889	32.298	14.544	50.441	1.00	27.37
1680	CD2	LEU	A	889	33.118	12.204	50.026	1.00	22.77
1681	N	TYR	A	890	29.048	12.255	52.874	1.00	19.92
1682	CA	TYR	A	890	27.668	12.011	52.439	1.00	19.47
1683	C	TYR	A	890	26.732	13.091	53.022	1.00	22.05
1684	O	TYR	A	890	25.853	13.637	52.339	1.00	20.67
1685	CB	TYR	A	890	27.237	10.601	52.890	1.00	19.20
1686	CG	TYR	A	890	25.944	10.124	52.272	1.00	27.69
1687	CD1	TYR	A	890	24.713	10.641	52.685	1.00	26.53
1688	CD2	TYR	A	890	25.954	9.174	51.250	1.00	24.52
1689	CE1	TYR	A	890	23.522	10.221	52.095	1.00	30.01
1690	CE2	TYR	A	890	24.773	8.751	50.654	1.00	26.75
1691	CZ	TYR	A	890	23.562	9.278	51.083	1.00	33.34
1692	OH	TYR	A	890	22.379	8.868	50.505	1.00	39.29
1693	N	CYS	A	891	26.938	13.417	54.291	1.00	19.66
1694	CA	CYS	A	891	26.129	14.427	54.968	1.00	21.68
1695	C	CYS	A	891	26.253	15.813	54.324	1.00	20.24
1696	O	CYS	A	891	25.256	16.468	54.016	1.00	22.45
1697	CB	CYS	A	891	26.547	14.505	56.440	1.00	22.87
1698	SG	CYS	A	891	25.632	15.719	57.423	1.00	25.25
1699	N	LEU	A	892	27.480	16.261	54.122	1.00	21.55
1700	CA	LEU	A	892	27.706	17.577	53.528	1.00	24.47
1701	C	LEU	A	892	27.148	17.649	52.110	1.00	25.40
1702	O	LEU	A	892	26.626	18.691	51.703	1.00	28.02
1703	CB	LEU	A	892	29.194	17.913	53.529	1.00	24.44
1704	CG	LEU	A	892	29.526	19.338	53.070	1.00	23.14

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1705	CD1	LEU	A	892	28.775	20.349	53.943	1.00	29.95
	1706	CD2	LEU	A	892	31.029	19.551	53.163	1.00	28.07
	1707	N	ASN	A	893	27.266	16.558	51.353	1.00	23.21
10	1708	CA	ASN	A	893	26.702	16.526	50.002	1.00	23.92
	1709	C	ASN	A	893	25.180	16.641	50.038	1.00	25.99
	1710	O	ASN	A	893	24.592	17.406	49.284	1.00	27.51
15	1711	CB	ASN	A	893	27.037	15.224	49.263	1.00	27.01
	1712	CG	ASN	A	893	28.363	15.275	48.562	1.00	29.03
	1713	OD1	ASN	A	893	28.794	16.335	48.109	1.00	30.83
20	1714	ND2	ASN	A	893	29.004	14.116	48.421	1.00	29.90
	1715	N	THR	A	894	24.543	15.853	50.896	1.00	25.80
	1716	CA	THR	A	894	23.089	15.871	51.014	1.00	25.04
25	1717	C	THR	A	894	22.594	17.211	51.529	1.00	24.51
	1718	O	THR	A	894	21.518	17.670	51.147	1.00	28.41
	1719	CB	THR	A	894	22.598	14.741	51.958	1.00	22.97
30	1720	OG1	THR	A	894	23.051	13.488	51.441	1.00	23.34
	1721	CG2	THR	A	894	21.089	14.729	52.057	1.00	25.92
	1722	N	PHE	A	895	23.395	17.832	52.390	1.00	23.12
35	1723	CA	PHE	A	895	23.072	19.126	52.983	1.00	23.28
	1724	C	PHE	A	895	23.083	20.188	51.878	1.00	26.81
	1725	O	PHE	A	895	22.185	21.022	51.808	1.00	27.75
40	1726	CB	PHE	A	895	24.113	19.477	54.049	1.00	22.97
	1727	CG	PHE	A	895	23.848	20.775	54.766	1.00	20.82
	1728	CD1	PHE	A	895	22.805	20.892	55.673	1.00	21.56
45	1729	CD2	PHE	A	895	24.632	21.892	54.497	1.00	25.72
	1730	CE1	PHE	A	895	22.536	22.104	56.310	1.00	26.99
	1731	CE2	PHE	A	895	24.374	23.109	55.126	1.00	28.83
50	1732	CZ	PHE	A	895	23.324	23.217	56.035	1.00	24.76
	1733	N	ILE	A	896	24.104	20.157	51.024	1.00	26.30
	1734	CA	ILE	A	896	24.189	21.112	49.915	1.00	27.51
55	1735	C	ILE	A	896	23.068	20.887	48.886	1.00	30.83
	1736	O	ILE	A	896	22.585	21.834	48.256	1.00	31.33
	1737	CB	ILE	A	896	25.561	21.018	49.213	1.00	30.94
55	1738	CG1	ILE	A	896	26.643	21.588	50.133	1.00	31.10
	1739	CG2	ILE	A	896	25.527	21.750	47.876	1.00	33.25
	1740	CD1	ILE	A	896	28.031	21.529	49.540	1.00	42.81
	1741	N	GLN	A	897	22.640	19.637	48.723	1.00	29.65

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1742	CA	GLN	A	897	21.590	19.326	47.752	1.00	30.69
1743	C	GLN	A	897	20.239	19.143	48.430	1.00	33.21
1744	O	GLN	A	897	19.288	18.673	47.800	1.00	36.42
1745	CB	GLN	A	897	21.951	18.040	47.003	1.00	34.22
1746	CG	GLN	A	897	23.385	18.025	46.508	1.00	33.58
1747	CD	GLN	A	897	23.814	16.698	45.900	1.00	46.71
1748	OE1	GLN	A	897	25.010	16.444	45.732	1.00	45.14
1749	NE2	GLN	A	897	22.847	15.857	45.547	1.00	39.95
1750	N	SER	A	898	20.145	19.519	49.705	1.00	31.45
1751	CA	SER	A	898	18.909	19.333	50.464	1.00	35.66
1752	C	SER	A	898	17.620	19.766	49.764	1.00	34.55
1753	O	SER	A	898	16.635	19.034	49.780	1.00	31.82
1754	CB	SER	A	898	19.011	20.008	51.839	1.00	32.53
1755	OG	SER	A	898	19.182	21.410	51.741	1.00	46.60
1756	N	ARG	A	899	17.606	20.942	49.149	1.00	37.58
1757	CA	ARG	A	899	16.385	21.377	48.482	1.00	43.27
1758	C	ARG	A	899	16.084	20.489	47.282	1.00	46.14
1759	O	ARG	A	899	14.925	20.152	47.023	1.00	46.04
1760	CB	ARG	A	899	16.488	22.847	48.057	1.00	45.98
1761	CG	ARG	A	899	16.891	23.785	49.194	1.00	58.17
1762	CD	ARG	A	899	16.030	23.598	50.451	1.00	63.03
1763	NE	ARG	A	899	14.637	24.028	50.302	1.00	72.16
1764	CZ	ARG	A	899	14.247	25.295	50.169	1.00	72.47
1765	NH1	ARG	A	899	15.142	26.275	50.168	1.00	73.96
1766	NH2	ARG	A	899	12.957	25.586	50.049	1.00	70.95
1767	N	ALA	A	900	17.127	20.076	46.571	1.00	43.89
1768	CA	ALA	A	900	16.960	19.227	45.400	1.00	44.86
1769	C	ALA	A	900	16.538	17.812	45.768	1.00	45.61
1770	O	ALA	A	900	15.768	17.174	45.053	1.00	44.57
1771	CB	ALA	A	900	18.260	19.181	44.601	1.00	49.14
1772	N	LEU	A	901	17.049	17.325	46.891	1.00	44.06
1773	CA	LEU	A	901	16.748	15.977	47.351	1.00	42.19
1774	C	LEU	A	901	15.509	15.927	48.227	1.00	40.67
1775	O	LEU	A	901	15.065	14.851	48.618	1.00	44.90
1776	CB	LEU	A	901	17.949	15.425	48.119	1.00	39.53
1777	CG	LEU	A	901	19.224	15.214	47.306	1.00	41.94
1778	CD1	LEU	A	901	20.369	14.833	48.234	1.00	43.72

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1779	CD2	LEU	A	901	18.984	14.128	46.266	1.00	41.21
	1780	N	SER	A	902	14.944	17.092	48.516	1.00	38.21
	1781	CA	SER	A	902	13.773	17.180	49.365	1.00	35.93
10	1782	C	SER	A	902	14.094	16.659	50.762	1.00	34.57
	1783	O	SER	A	902	13.243	16.063	51.415	1.00	33.32
	1784	CB	SER	A	902	12.603	16.382	48.773	1.00	42.40
15	1785	OG	SER	A	902	12.170	16.942	47.546	1.00	50.36
	1786	N	VAL	A	903	15.325	16.884	51.219	1.00	32.92
	1787	CA	VAL	A	903	15.734	16.436	52.552	1.00	30.26
20	1788	C	VAL	A	903	15.849	17.645	53.484	1.00	31.81
	1789	O	VAL	A	903	16.582	18.586	53.198	1.00	34.09
	1790	CB	VAL	A	903	17.087	15.700	52.500	1.00	30.61
25	1791	CG1	VAL	A	903	17.527	15.298	53.919	1.00	30.31
	1792	CG2	VAL	A	903	16.967	14.449	51.608	1.00	26.90
	1793	N	GLU	A	904	15.104	17.627	54.584	1.00	28.12
30	1794	CA	GLU	A	904	15.153	18.720	55.543	1.00	27.45
	1795	C	GLU	A	904	16.163	18.489	56.665	1.00	27.94
	1796	O	GLU	A	904	16.217	17.400	57.223	1.00	26.23
35	1797	CB	GLU	A	904	13.780	18.941	56.175	1.00	33.68
	1798	CG	GLU	A	904	13.807	20.006	57.271	1.00	51.81
	1799	CD	GLU	A	904	12.457	20.233	57.929	1.00	62.71
40	1800	OE1	GLU	A	904	11.469	19.575	57.530	1.00	63.38
	1801	OE2	GLU	A	904	12.387	21.080	58.852	1.00	63.52
	1802	N	PHE	A	905	16.957	19.516	56.982	1.00	25.35
45	1803	CA	PHE	A	905	17.935	19.447	58.071	1.00	24.39
	1804	C	PHE	A	905	17.468	20.454	59.109	1.00	26.69
	1805	O	PHE	A	905	17.219	21.610	58.770	1.00	27.33
50	1806	CB	PHE	A	905	19.359	19.856	57.629	1.00	25.14
	1807	CG	PHE	A	905	20.072	18.833	56.786	1.00	21.63
	1808	CD1	PHE	A	905	19.735	18.642	55.457	1.00	22.11
55	1809	CD2	PHE	A	905	21.068	18.043	57.343	1.00	23.38
	1810	CE1	PHE	A	905	20.383	17.678	54.691	1.00	19.55
	1811	CE2	PHE	A	905	21.726	17.072	56.592	1.00	24.14
55	1812	CZ	PHE	A	905	21.382	16.888	55.261	1.00	22.83
	1813	N	PRO	A	906	17.333	20.037	60.379	1.00	23.73
	1814	CA	PRO	A	906	16.891	20.955	61.432	1.00	22.74
	1815	C	PRO	A	906	17.982	22.002	61.720	1.00	22.33

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1816	O	PRO	A	906	19.116	21.882	61.267	1.00	22.26
1817	CB	PRO	A	906	16.649	20.024	62.623	1.00	24.51
1818	CG	PRO	A	906	16.392	18.675	61.959	1.00	30.94
1819	CD	PRO	A	906	17.516	18.695	60.948	1.00	29.32
1820	N	GLU	A	907	17.627	23.016	62.495	1.00	25.11
1821	CA	GLU	A	907	18.543	24.119	62.809	1.00	22.58
1822	C	GLU	A	907	19.848	23.834	63.543	1.00	21.81
1823	O	GLU	A	907	20.896	24.342	63.162	1.00	23.58
1824	CB	GLU	A	907	17.782	25.193	63.589	1.00	23.00
1825	CG	GLU	A	907	16.592	25.833	62.848	1.00	25.08
1826	CD	GLU	A	907	16.951	26.530	61.539	1.00	31.26
1827	OE1	GLU	A	907	18.064	27.086	61.413	1.00	31.56
1828	OE2	GLU	A	907	16.089	26.561	60.631	1.00	31.17
1829	N	MET	A	908	19.803	23.052	64.618	1.00	20.50
1830	CA	MET	A	908	21.033	22.786	65.356	1.00	22.40
1831	C	MET	A	908	21.994	21.936	64.541	1.00	20.88
1832	O	MET	A	908	23.205	22.153	64.566	1.00	22.84
1833	CB	MET	A	908	20.706	22.112	66.694	1.00	28.13
1834	CG	MET	A	908	19.770	22.954	67.553	1.00	30.10
1835	SD	MET	A	908	19.342	22.226	69.147	1.00	36.75
1836	CE	MET	A	908	18.819	20.575	68.656	1.00	29.48
1837	N	MET	A	909	21.458	20.977	63.798	1.00	22.18
1838	CA	MET	A	909	22.303	20.120	62.982	1.00	20.40
1839	C	MET	A	909	22.866	20.915	61.825	1.00	20.24
1840	O	MET	A	909	24.018	20.734	61.442	1.00	20.23
1841	CB	MET	A	909	21.496	18.937	62.450	1.00	24.51
1842	CG	MET	A	909	22.335	17.920	61.747	1.00	36.88
1843	SD	MET	A	909	21.313	16.481	61.357	1.00	38.44
1844	CE	MET	A	909	22.491	15.495	60.507	1.00	42.73
1845	N	SER	A	910	22.052	21.801	61.263	1.00	22.17
1846	CA	SER	A	910	22.520	22.624	60.160	1.00	24.13
1847	C	SER	A	910	23.678	23.505	60.651	1.00	24.76
1848	O	SER	A	910	24.641	23.752	59.915	1.00	20.25
1849	CB	SER	A	910	21.381	23.509	59.630	1.00	24.96
1850	OG	SER	A	910	20.334	22.728	59.067	1.00	29.09
1851	N	GLU	A	911	23.577	23.985	61.888	1.00	21.90
1852	CA	GLU	A	911	24.637	24.831	62.430	1.00	25.07

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1853	C	GLU	A	911	25.965	24.103	62.594	1.00	25.56
1854	O	GLU	A	911	26.997	24.631	62.208	1.00	26.95
1855	CB	GLU	A	911	24.232	25.458	63.770	1.00	26.93
1856	CG	GLU	A	911	25.361	26.272	64.407	1.00	30.33
1857	CD	GLU	A	911	25.842	27.437	63.535	1.00	45.68
1858	OE1	GLU	A	911	25.054	27.944	62.705	1.00	48.37
1859	OE2	GLU	A	911	27.010	27.865	63.694	1.00	40.75
1860	N	VAL	A	912	25.959	22.901	63.163	1.00	23.66
1861	CA	VAL	A	912	27.215	22.197	63.335	1.00	24.09
1862	C	VAL	A	912	27.816	21.806	61.995	1.00	22.11
1863	O	VAL	A	912	29.035	21.848	61.830	1.00	23.47
1864	CB	VAL	A	912	27.070	20.931	64.259	1.00	25.40
1865	CG1	VAL	A	912	26.617	21.357	65.635	1.00	27.52
1866	CG2	VAL	A	912	26.066	19.926	63.673	1.00	28.29
1867	N	ILE	A	913	26.968	21.462	61.022	1.00	20.76
1868	CA	ILE	A	913	27.475	21.077	59.704	1.00	20.13
1869	C	ILE	A	913	28.167	22.255	59.050	1.00	23.37
1870	O	ILE	A	913	29.302	22.149	58.567	1.00	25.36
1871	CB	ILE	A	913	26.336	20.565	58.788	1.00	19.24
1872	CG1	ILE	A	913	25.835	19.220	59.302	1.00	22.39
1873	CG2	ILE	A	913	26.833	20.425	57.348	1.00	18.20
1874	CD1	ILE	A	913	24.472	18.815	58.727	1.00	26.26
1875	N	ALA	A	914	27.491	23.392	59.051	1.00	23.60
1876	CA	ALA	A	914	28.041	24.600	58.451	1.00	30.05
1877	C	ALA	A	914	29.260	25.131	59.199	1.00	27.97
1878	O	ALA	A	914	30.189	25.666	58.595	1.00	31.89
1879	CB	ALA	A	914	26.953	25.694	58.381	1.00	24.81
1880	N	ALA	A	915	29.273	24.983	60.515	1.00	28.98
1881	CA	ALA	A	915	30.394	25.494	61.292	1.00	30.10
1882	C	ALA	A	915	31.698	24.711	61.143	1.00	29.70
1883	O	ALA	A	915	32.777	25.299	61.203	1.00	30.09
1884	CB	ALA	A	915	30.009	25.578	62.773	1.00	29.66
1885	N	GLN	A	916	31.622	23.401	60.923	1.00	26.34
1886	CA	GLN	A	916	32.848	22.627	60.843	1.00	23.29
1887	C	GLN	A	916	33.045	21.567	59.764	1.00	23.47
1888	O	GLN	A	916	34.190	21.219	59.480	1.00	24.44
1889	CB	GLN	A	916	33.101	21.914	62.180	1.00	29.83

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
1890	CG	GLN	A	916	33.182	22.761	63.424	1.00	31.14
1891	CD	GLN	A	916	34.230	23.845	63.355	1.00	37.37
1892	OE1	GLN	A	916	35.302	23.660	62.780	1.00	33.07
1893	NE2	GLN	A	916	33.938	24.979	63.979	1.00	42.40
1894	N	LEU	A	917	31.980	21.005	59.193	1.00	24.92
1895	CA	LEU	A	917	32.200	19.927	58.218	1.00	27.91
1896	C	LEU	A	917	33.163	20.194	57.078	1.00	27.51
1897	O	LEU	A	917	34.019	19.362	56.790	1.00	30.01
1898	CB	LEU	A	917	30.885	19.372	57.646	1.00	28.45
1899	CG	LEU	A	917	30.195	18.339	58.540	1.00	34.41
1900	CD1	LEU	A	917	29.179	17.522	57.722	1.00	28.16
1901	CD2	LEU	A	917	31.244	17.388	59.093	1.00	34.26
1902	N	PRO	A	918	33.025	21.329	56.387	1.00	27.54
1903	CA	PRO	A	918	33.977	21.564	55.301	1.00	27.73
1904	C	PRO	A	918	35.434	21.568	55.809	1.00	24.86
1905	O	PRO	A	918	36.325	21.024	55.166	1.00	25.75
1906	CB	PRO	A	918	33.536	22.922	54.762	1.00	27.68
1907	CG	PRO	A	918	32.031	22.901	55.026	1.00	26.00
1908	CD	PRO	A	918	32.060	22.439	56.472	1.00	28.16
1909	N	LYS	A	919	35.672	22.184	56.962	1.00	23.19
1910	CA	LYS	A	919	37.023	22.238	57.529	1.00	24.99
1911	C	LYS	A	919	37.508	20.830	57.870	1.00	26.95
1912	O	LYS	A	919	38.632	20.444	57.537	1.00	26.77
1913	CB	LYS	A	919	37.023	23.105	58.794	1.00	31.71
1914	CG	LYS	A	919	38.382	23.291	59.446	1.00	36.39
1915	CD	LYS	A	919	38.233	24.038	60.774	1.00	41.59
1916	CE	LYS	A	919	37.608	25.418	60.579	1.00	46.46
1917	NZ	LYS	A	919	37.319	26.115	61.879	1.00	52.55
1918	N	ILE	A	920	36.655	20.057	58.533	1.00	25.62
1919	CA	ILE	A	920	37.013	18.683	58.898	1.00	25.44
1920	C	ILE	A	920	37.322	17.851	57.660	1.00	28.84
1921	O	ILE	A	920	38.336	17.156	57.607	1.00	23.14
1922	CB	ILE	A	920	35.871	18.019	59.665	1.00	25.43
1923	CG1	ILE	A	920	35.618	18.810	60.951	1.00	27.84
1924	CG2	ILE	A	920	36.195	16.555	59.947	1.00	26.23
1925	CD1	ILE	A	920	34.396	18.353	61.713	1.00	30.88
1926	N	LEU	A	921	36.439	17.900	56.667	1.00	26.45

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	1964	CD	LYS	A	926	47.144	17.464	66.576	1.00	42.65
	1965	CE	LYS	A	926	48.016	16.489	67.350	1.00	45.66
	1966	NZ	LYS	A	926	48.834	15.673	66.424	1.00	41.46
10	1967	N	PRO	A	927	43.494	14.725	63.825	1.00	29.35
	1968	CA	PRO	A	927	42.894	13.504	64.360	1.00	29.76
	1969	C	PRO	A	927	43.890	12.891	65.342	1.00	32.65
15	1970	O	PRO	A	927	45.079	12.817	65.033	1.00	31.57
	1971	CB	PRO	A	927	42.721	12.641	63.109	1.00	32.15
	1972	CG	PRO	A	927	42.704	13.692	61.952	1.00	33.46
20	1973	CD	PRO	A	927	43.837	14.547	62.404	1.00	29.87
	1974	N	LEU	A	928	43.442	12.483	66.528	1.00	26.08
	1975	CA	LEU	A	928	44.376	11.871	67.467	1.00	28.80
25	1976	C	LEU	A	928	44.318	10.382	67.226	1.00	32.70
	1977	O	LEU	A	928	43.235	9.805	67.126	1.00	32.54
	1978	CB	LEU	A	928	44.005	12.198	68.920	1.00	28.21
30	1979	CG	LEU	A	928	43.999	13.703	69.214	1.00	27.44
	1980	CD1	LEU	A	928	43.689	13.946	70.690	1.00	25.95
	1981	CD2	LEU	A	928	45.361	14.305	68.852	1.00	28.60
35	1982	N	LEU	A	929	45.485	9.763	67.116	1.00	29.11
	1983	CA	LEU	A	929	45.564	8.329	66.855	1.00	32.04
	1984	C	LEU	A	929	46.301	7.595	67.966	1.00	33.98
40	1985	O	LEU	A	929	47.258	8.125	68.526	1.00	35.14
	1986	CB	LEU	A	929	46.292	8.092	65.525	1.00	30.80
	1987	CG	LEU	A	929	45.639	8.707	64.281	1.00	41.73
45	1988	CD1	LEU	A	929	46.568	8.573	63.076	1.00	37.07
	1989	CD2	LEU	A	929	44.309	8.022	64.023	1.00	38.20
	1990	N	PHE	A	930	45.844	6.387	68.293	1.00	30.93
50	1991	CA	PHE	A	930	46.505	5.580	69.316	1.00	36.94
	1992	C	PHE	A	930	47.659	4.788	68.730	1.00	37.82
	1993	O	PHE	A	930	48.595	4.419	69.441	1.00	40.73
55	1994	CB	PHE	A	930	45.546	4.589	69.962	1.00	33.98
	1995	CG	PHE	A	930	44.615	5.212	70.942	1.00	31.86
	1996	CD1	PHE	A	930	45.035	5.440	72.248	1.00	27.98
	1997	CD2	PHE	A	930	43.346	5.613	70.562	1.00	29.84
	1998	CE1	PHE	A	930	44.197	6.063	73.157	1.00	34.01
	1999	CE2	PHE	A	930	42.496	6.238	71.470	1.00	31.12
	2000	CZ	PHE	A	930	42.922	6.464	72.765	1.00	31.58

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2038	C17	STR	A	1	22.714	11.149	56.627	1.00	22.28
2039	C18	STR	A	1	23.659	12.677	58.454	1.00	20.57
2040	C19	STR	A	1	23.427	11.246	63.007	1.00	21.41
2041	C20	STR	A	1	22.375	12.388	55.781	1.00	25.07
2042	O20	STR	A	1	23.212	12.876	55.052	1.00	29.48
2043	C21	STR	A	1	21.009	12.976	55.857	1.00	25.63
2044	N	LEU	B	683	60.447	28.744	14.730	1.00	61.24
2045	CA	LEU	B	683	59.070	29.295	14.876	1.00	59.60
2046	C	LEU	B	683	58.273	28.573	15.963	1.00	56.34
2047	O	LEU	B	683	58.751	27.612	16.566	1.00	58.01
2048	CB	LEU	B	683	58.346	29.241	13.523	1.00	59.47
2049	CG	LEU	B	683	58.334	27.934	12.719	1.00	63.19
2050	CD1	LEU	B	683	57.530	26.865	13.447	1.00	61.93
2051	CD2	LEU	B	683	57.728	28.201	11.343	1.00	61.94
2052	N	ILE	B	684	57.055	29.045	16.212	1.00	57.02
2053	CA	ILE	B	684	56.194	28.468	17.244	1.00	48.99
2054	C	ILE	B	684	55.519	27.152	16.828	1.00	48.76
2055	O	ILE	B	684	54.990	27.044	15.724	1.00	41.43
2056	CB	ILE	B	684	55.094	29.468	17.631	1.00	54.99
2057	CG1 I	ILE	B	684	55.718	30.827	17.971	1.00	54.78
2058	CG2	ILE	B	684	54.296	28.933	18.815	1.00	49.74
2059	CD1	ILE	B	684	56.677	30.804	19.143	1.00	54.94
2060	N	PRO	B	685	55.532	26.135	17.710	1.00	42.36
2061	CA	PRO	B	685	54.912	24.837	17.424	1.00	42.23
2062	C	PRO	B	685	53.443	25.058	17.084	1.00	41.20
2063	O	PRO	B	685	52.741	25.801	17.780	1.00	37.15
2064	CB	PRO	B	685	55.095	24.082	18.738	1.00	44.89
2065	CG	PRO	B	685	56.412	24.638	19.230	1.00	47.57
2066	CD	PRO	B	685	56.116	26.115	19.062	1.00	46.29
2067	N	PRO	B	686	52.948	24.395	16.029	1.00	37.46
2068	CA	PRO	B	686	51.549	24.575	15.644	1.00	35.10
2069	C	PRO	B	686	50.533	24.458	16.783	1.00	29.47
2070	O	PRO	B	686	49.675	25.317	16.919	1.00	28.34
2071	CB	PRO	B	686	51.364	23.520	14.549	1.00	37.20
2072	CG	PRO	B	686	52.417	22.466	14.906	1.00	39.30
2073	CD	PRO	B	686	53.579	23.402	15.146	1.00	39.17
2074	N	LEU	B	687	50.641	23.423	17.607	1.00	27.64

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2075	CA	LEU	B	687	49.680	23.254	18.698	1.00	29.33
	2076	C	LEU	B	687	49.656	24.470	19.623	1.00	32.07
	2077	O	LEU	B	687	48.603	24.851	20.154	1.00	29.30
10	2078	CB	LEU	B	687	49.991	21.982	19.489	1.00	29.35
	2079	CG	LEU	B	687	49.030	21.634	20.640	1.00	28.23
	2080	CD1	LEU	B	687	47.590	21.521	20.135	1.00	34.54
15	2081	CD2	LEU	B	687	49.476	20.327	21.279	1.00	37.01
	2082	N	ILE	B	688	50.814	25.094	19.810	1.00	29.32
	2083	CA	ILE	B	688	50.893	26.268	20.659	1.00	29.95
20	2084	C	ILE	B	688	50.225	27.466	19.976	1.00	29.12
	2085	O	ILE	B	688	49.544	28.260	20.626	1.00	31.19
	2086	CB	ILE	B	688	52.365	26.573	21.029	1.00	25.50
25	2087	CG1	ILE	B	688	52.945	25.393	21.826	1.00	35.36
	2088	CG2	ILE	B	688	52.450	27.851	21.831	1.00	30.73
	2089	CD1	ILE	B	688	54.354	25.613	22.354	1.00	30.80
30	2090	N	ASN	B	689	50.396	27.607	18.663	1.00	32.90
	2091	CA	ASN	B	689	49.744	28.720	17.970	1.00	26.76
	2092	C	ASN	B	689	48.246	28.520	18.037	1.00	27.49
35	2093	O	ASN	B	689	47.490	29.473	18.168	1.00	29.38
	2094	CB	ASN	B	689	50.163	28.802	16.497	1.00	37.63
	2095	CG	ASN	B	689	51.544	29.392	16.315	1.00	42.51
40	2096	OD1	ASN	B	689	51.843	30.467	16.844	1.00	50.26
	2097	ND2	ASN	B	689	52.391	28.706	15.550	1.00	49.44
	2098	N	LEU	B	690	47.816	27.270	17.938	1.00	26.48
45	2099	CA	LEU	B	690	46.389	26.992	17.998	1.00	30.44
	2100	C	LEU	B	690	45.879	27.386	19.379	1.00	29.46
	2101	O	LEU	B	690	44.849	28.034	19.487	1.00	25.83
50	2102	CB	LEU	B	690	46.110	25.518	17.737	1.00	33.45
	2103	CG	LEU	B	690	44.641	25.073	17.699	1.00	36.64
	2104	CD1	LEU	B	690	43.832	25.943	16.752	1.00	48.71
55	2105	CD2	LEU	B	690	44.591	23.624	17.254	1.00	48.02
	2106	N	LEU	B	691	46.607	26.999	20.426	1.00	24.64
	2107	CA	LEU	B	691	46.203	27.342	21.788	1.00	25.80
55	2108	C	LEU	B	691	46.058	28.845	21.954	1.00	24.20
	2109	O	LEU	B	691	45.139	29.311	22.620	1.00	27.02
	2110	CB	LEU	B	691	47.195	26.774	22.821	1.00	23.63
	2111	CG	LEU	B	691	47.230	25.246	23.002	1.00	27.81

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2112	CD1	LEU	B	691	48.278	24.847	24.069	1.00	22.95
2113	CD2	LEU	B	691	45.838	24.749	23.443	1.00	24.81
2114	N	MET	B	692	46.942	29.626	21.337	1.00	27.01
2115	CA	MET	B	692	46.833	31.077	21.464	1.00	28.55
2116	C	MET	B	692	45.605	31.584	20.723	1.00	28.03
2117	O	MET	B	692	44.955	32.535	21.154	1.00	29.01
2118	CB	MET	B	692	48.086	31.780	20.922	1.00	34.30
2119	CG	MET	B	692	48.009	33.297	21.034	1.00	43.26
2120	SD	MET	B	692	47.662	33.855	22.730	1.00	60.38
2121	CE	MET	B	692	47.493	35.639	22.492	1.00	57.28
2122	N	SER	B	693	45.300	30.936	19.609	1.00	30.34
2123	CA	SER	B	693	44.153	31.288	18.782	1.00	33.29
2124	C	SER	B	693	42.802	31.154	19.478	1.00	31.49
2125	O	SER	B	693	41.906	31.971	19.269	1.00	31.71
2126	CB	SER	B	693	44.140	30.404	17.534	1.00	35.00
2127	OG	SER	B	693	42.924	30.567	16.829	1.00	53.17
2128	N	ILE	B	694	42.652	30.124	20.308	1.00	30.50
2129	CA	ILE	B	694	41.380	29.891	20.983	1.00	29.73
2130	C	ILE	B	694	41.282	30.457	22.389	1.00	29.02
2131	O	ILE	B	694	40.279	30.258	23.066	1.00	27.58
2132	CB	ILE	B	694	41.043	28.375	21.043	1.00	28.72
2133	CG1	ILE	B	694	42.051	27.648	21.929	1.00	26.83
2134	CG2	ILE	B	694	41.070	27.780	19.626	1.00	26.41
2135	CD1	ILE	B	694	41.753	26.158	22.140	1.00	25.75
2136	N	GLU	B	695	42.318	31.160	22.832	1.00	28.38
2137	CA	GLU	B	695	42.300	31.744	24.166	1.00	34.30
2138	C	GLU	B	695	41.148	32.745	24.219	1.00	32.52
2139	O	GLU	B	695	40.968	33.533	23.302	1.00	40.33
2140	CB	GLU	B	695	43.609	32.484	24.445	1.00	34.44
2141	CG	GLU	B	695	43.717	32.959	25.870	1.00	44.19
2142	CD	GLU	B	695	44.179	31.868	26.819	1.00	46.10
2143	OE1	GLU	B	695	43.742	30.701	26.682	1.00	34.62
2144	OE2	GLU	B	695	44.983	32.196	27.718	1.00	55.08
2145	N	PRO	B	696	40.353	32.729	25.298	1.00	35.67
2146	CA	PRO	B	696	39.216	33.642	25.460	1.00	33.01
2147	C	PRO	B	696	39.590	35.124	25.452	1.00	38.74
2148	O	PRO	B	696	40.695	35.502	25.834	1.00	31.49

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2149	CB	PRO	B	696	38.633	33.216	26.808	1.00	33.87
2150	CG	PRO	B	696	38.988	31.725	26.849	1.00	42.63
2151	CD	PRO	B	696	40.449	31.833	26.461	1.00	33.91
2152	N	ASP	B	697	38.660	35.961	25.016	1.00	37.09
2153	CA	ASP	B	697	38.896	37.392	24.995	1.00	40.83
2154	C	ASP	B	697	38.697	37.865	26.445	1.00	41.22
2155	O	ASP	B	697	38.208	37.108	27.281	1.00	31.86
2156	CB	ASP	B	697	37.881	38.064	24.070	1.00	51.77
2157	CG	ASP	B	697	38.345	39.419	23.581	1.00	50.70
2158	OD1	ASP	B	697	38.620	40.306	24.416	1.00	65.14
2159	OD2	ASP	B	697	38.437	39.595	22.352	1.00	58.30
2160	N	VAL	B	698	39.086	39.099	26.752	1.00	40.92
2161	CA	VAL	B	698	38.925	39.600	28.115	1.00	39.77
2162	C	VAL	B	698	37.462	39.569	28.523	1.00	36.77
2163	O	VAL	B	698	36.567	39.817	27.710	1.00	39.48
2164	CB	VAL	B	698	39.463	41.044	28.271	1.00	47.15
2165	CG1	VAL	B	698	40.986	41.049	28.157	1.00	51.98
2166	CG2	VAL	B	698	38.851	41.948	27.206	1.00	44.01
2167	N	ILE	B	699	37.216	39.238	29.784	1.00	34.12
2168	CA	ILE	B	699	35.857	39.178	30.305	1.00	25.82
2169	C	ILE	B	699	35.728	40.202	31.421	1.00	30.49
2170	O	ILE	B	699	36.616	40.315	32.264	1.00	26.57
2171	CB	ILE	B	699	35.550	37.758	30.841	1.00	28.35
2172	CG1	ILE	B	699	35.595	36.770	29.677	1.00	28.39
2173	CG2	ILE	B	699	34.198	37.731	31.553	1.00	25.63
2174	CD1	ILE	B	699	35.451	35.322	30.072	1.00	35.91
2175	N	TYR	B	700	34.631	40.956	31.408	1.00	29.91
2176	CA	TYR	B	700	34.369	41.975	32.422	1.00	32.17
2177	C	TYR	B	700	33.522	41.412	33.561	1.00	32.19
2178	O	TYR	B	700	32.717	40.511	33.357	1.00	33.61
2179	CB	TYR	B	700	33.629	43.152	31.793	1.00	37.36
2180	CG	TYR	B	700	34.433	43.900	30.760	1.00	44.51
2181	CD1	TYR	B	700	35.387	44.848	31.134	1.00	48.38
2182	CD2	TYR	B	700	34.267	43.635	29.402	1.00	49.71
2183	CE1	TYR	B	700	36.154	45.515	30.170	1.00	52.90
2184	CE2	TYR	B	700	35.025	44.290	28.438	1.00	52.02
2185	CZ	TYR	B	700	35.966	45.227	28.823	1.00	54.03

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2186	OH	TYR	B	700	36.721	45.862	27.854	1.00	59.25
2187	N	ALA	B	701	33.695	41.962	34.757	1.00	30.94
2188	CA	ALA	B	701	32.938	41.509	35.919	1.00	33.53
2189	C	ALA	B	701	31.571	42.184	36.006	1.00	36.38
2190	O	ALA	B	701	30.657	41.664	36.657	1.00	33.68
2191	CB	ALA	B	701	33.730	41.787	37.204	1.00	30.56
2192	N	GLY	B	702	31.435	43.333	35.344	1.00	34.92
2193	CA	GLY	B	702	30.192	44.082	35.396	1.00	36.02
2194	C	GLY	B	702	30.048	44.717	36.766	1.00	36.08
2195	O	GLY	B	702	28.944	44.994	37.224	1.00	35.67
2196	N	HIS	B	703	31.178	44.967	37.419	1.00	36.94
2197	CA	HIS	B	703	31.181	45.536	38.759	1.00	39.32
2198	C	HIS	B	703	30.955	47.049	38.842	1.00	43.22
2199	O	HIS	B	703	31.440	47.806	38.010	1.00	37.01
2200	CB	HIS	B	703	32.486	45.158	39.460	1.00	38.71
2201	CG	HIS	B	703	32.561	45.614	40.881	1.00	36.27
2202	ND1	HIS	B	703	32.950	46.888	41.232	1.00	43.46
2203	CD2	HIS	B	703	32.243	44.985	42.035	1.00	36.91
2204	CE1	HIS	B	703	32.870	47.024	42.543	1.00	38.85
2205	NE2	HIS	B	703	32.442	45.882	43.054	1.00	41.40
2206	N	ASP	B	704	30.221	47.471	39.871	1.00	46.40
2207	CA	ASP	B	704	29.898	48.880	40.097	1.00	53.26
2208	C	ASP	B	704	31.066	49.860	39.983	1.00	53.35
2209	O	ASP	B	704	31.280	50.462	38.932	1.00	58.50
2210	CB	ASP	B	704	29.229	49.051	41.470	1.00	61.65
2211	CG	ASP	B	704	30.001	48.370	42.592	1.00	66.85
2212	OD1	ASP	B	704	30.031	47.119	42.619	1.00	72.50
2213	OD2	ASP	B	704	30.580	49.082	43.441	1.00	69.65
2214	N	ASN	B	705	31.809	50.011	41.074	1.00	55.13
2215	CA	ASN	B	705	32.951	50.922	41.157	1.00	50.42
2216	C	ASN	B	705	32.525	52.345	41.457	1.00	54.10
2217	O	ASN	B	705	33.359	53.174	41.812	1.00	52.31
2218	CB	ASN	B	705	33.805	50.915	39.882	1.00	52.40
2219	CG	ASN	B	705	34.614	49.646	39.729	1.00	47.64
2220	OD1	ASN	B	705	35.296	49.218	40.661	1.00	49.26
2221	ND2	ASN	B	705	34.555	49.043	38.546	1.00	47.16
2222	N	THR	B	706	31.236	52.637	41.308	1.00	52.08

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2260	N	SER	B	711	31.971	43.605	51.598	1.00	36.89
2261	CA	SER	B	711	32.320	42.200	51.449	1.00	43.49
2262	C	SER	B	711	31.361	41.476	50.522	1.00	41.27
2263	O	SER	B	711	31.780	40.718	49.647	1.00	43.17
2264	CB	SER	B	711	32.304	41.500	52.807	1.00	40.05
2265	OG	SER	B	711	32.541	40.115	52.642	1.00	53.25
2266	N	SER	B	712	30.069	41.717	50.709	1.00	40.73
2267	CA	SER	B	712	29.069	41.041	49.897	1.00	38.79
2268	C	SER	B	712	29.018	41.457	48.434	1.00	37.75
2269	O	SER	B	712	28.812	40.601	47.578	1.00	32.93
2270	CB	SER	B	712	27.680	41.185	50.528	1.00	40.76
2271	OG	SER	B	712	27.288	42.541	50.611	1.00	52.08
2272	N	SER	B	713	29.207	42.744	48.136	1.00	31.42
2273	CA	SER	B	713	29.151	43.196	46.744	1.00	30.39
2274	C	SER	B	713	30.384	42.769	45.962	1.00	26.79
2275	O	SER	B	713	30.287	42.444	44.787	1.00	27.38
2276	CB	SER	B	713	28.991	44.725	46.651	1.00	32.46
2277	OG	SER	B	713	30.115	45.404	47.190	1.00	37.41
2278	N	LEU	B	714	31.539	42.777	46.620	1.00	26.90
2279	CA	LEU	B	714	32.796	42.386	45.989	1.00	23.45
2280	C	LEU	B	714	32.815	40.878	45.691	1.00	25.66
2281	O	LEU	B	714	33.186	40.465	44.592	1.00	24.25
2282	CB	LEU	B	714	33.959	42.750	46.908	1.00	30.39
2283	CG	LEU	B	714	35.393	42.649	46.411	1.00	38.20
2284	CD1	LEU	B	714	35.557	43.398	45.091	1.00	41.76
2285	CD2	LEU	B	714	36.309	43.239	47.491	1.00	35.78
2286	N	LEU	B	715	32.436	40.055	46.666	1.00	20.32
2287	CA	LEU	B	715	32.409	38.607	46.435	1.00	24.51
2288	C	LEU	B	715	31.303	38.257	45.423	1.00	23.41
2289	O	LEU	B	715	31.449	37.350	44.615	1.00	19.77
2290	CB	LEU	B	715	32.219	37.855	47.757	1.00	23.31
2291	CG	LEU	B	715	33.439	37.895	48.691	1.00	25.25
2292	CD1	LEU	B	715	33.075	37.397	50.065	1.00	26.50
2293	CD2	LEU	B	715	34.583	37.067	48.089	1.00	22.19
2294	N	THR	B	716	30.204	38.998	45.447	1.00	22.64
2295	CA	THR	B	716	29.123	38.728	44.496	1.00	23.68
2296	C	THR	B	716	29.605	39.054	43.073	1.00	22.06

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2334	C	LEU	B	721	33.197	35.652	36.683	1.00	23.82
	2335	O	LEU	B	721	33.417	35.172	35.566	1.00	22.42
	2336	CB	LEU	B	721	34.096	37.866	37.498	1.00	21.95
10	2337	CG	LEU	B	721	35.387	37.769	36.696	1.00	20.86
	2338	CD1	LEU	B	721	35.162	38.452	35.346	1.00	22.61
	2339	CD2	LEU	B	721	36.537	38.433	37.453	1.00	19.99
15	2340	N	GLY	B	722	33.219	34.925	37.793	1.00	18.60
	2341	CA	GLY	B	722	33.464	33.495	37.739	1.00	21.51
	2342	C	GLY	B	722	32.497	32.793	36.807	1.00	22.85
20	2343	O	GLY	B	722	32.888	31.928	36.019	1.00	21.10
	2344	N	GLU	B	723	31.225	33.174	36.889	1.00	20.92
	2345	CA	GLU	B	723	30.187	32.582	36.044	1.00	22.44
25	2346	C	GLU	B	723	30.514	32.814	34.570	1.00	22.88
	2347	O	GLU	B	723	30.448	31.895	33.766	1.00	22.34
	2348	CB	GLU	B	723	28.830	33.219	36.370	1.00	28.49
30	2349	CG	GLU	B	723	27.635	32.646	35.614	1.00	29.16
	2350	CD	GLU	B	723	27.225	31.269	36.108	1.00	48.36
	2351	OE1	GLU	B	723	28.005	30.666	36.876	1.00	43.10
35	2352	OE2	GLU	B	723	26.126	30.784	35.726	1.00	39.94
	2353	N	ARG	B	724	30.858	34.054	34.225	1.00	20.90
	2354	CA	ARG	B	724	31.185	34.389	32.846	1.00	24.02
40	2355	C	ARG	B	724	32.431	33.652	32.389	1.00	24.96
	2356	O	ARG	B	724	32.512	33.179	31.260	1.00	21.65
	2357	CB	ARG	B	724	31.417	35.884	32.712	1.00	27.26
45	2358	CG	ARG	B	724	30.227	36.735	33.040	1.00	26.22
	2359	CD	ARG	B	724	30.661	38.187	33.084	1.00	29.11
	2360	NE	ARG	B	724	29.636	39.091	33.592	1.00	39.88
50	2361	CZ	ARG	B	724	28.566	39.475	32.905	1.00	47.37
	2362	NH1	ARG	B	724	28.370	39.029	31.668	1.00	54.23
	2363	NH2	ARG	B	724	27.708	40.329	33.445	1.00	44.85
55	2364	N	GLN	B	725	33.419	33.573	33.267	1.00	20.98
	2365	CA	GLN	B	725	34.631	32.866	32.910	1.00	24.59
	2366	C	GLN	B	725	34.372	31.378	32.750	1.00	26.24
55	2367	O	GLN	B	725	35.002	30.735	31.912	1.00	23.92
	2368	CB	GLN	B	725	35.712	33.097	33.958	1.00	22.57
	2369	CG	GLN	B	725	36.411	34.427	33.771	1.00	29.09
	2370	CD	GLN	B	725	37.471	34.675	34.813	1.00	34.68

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2371	OE1	GLN	B	725	38.060	33.730	35.349	1.00	34.94
	2372	NE2	GLN	B	725	37.749	35.944	35.089	1.00	31.50
	2373	N	LEU	B	726	33.452	30.834	33.544	1.00	22.27
10	2374	CA	LEU	B	726	33.141	29.411	33.450	1.00	22.12
	2375	C	LEU	B	726	32.524	29.133	32.077	1.00	22.14
	2376	O	LEU	B	726	32.838	28.124	31.433	1.00	19.87
15	2377	CB	LEU	B	726	32.197	28.991	34.585	1.00	21.36
	2378	CG	LEU	B	726	31.870	27.503	34.717	1.00	28.83
	2379	CD1	LEU	B	726	33.166	26.696	34.750	1.00	26.29
20	2380	CD2	LEU	B	726	31.042	27.265	35.999	1.00	27.99
	2381	N	LEU	B	727	31.652	30.023	31.619	1.00	21.02
	2382	CA	LEU	B	727	31.059	29.837	30.301	1.00	25.96
25	2383	C	LEU	B	727	32.150	29.841	29.230	1.00	25.51
	2384	O	LEU	B	727	32.080	29.064	28.266	1.00	20.92
	2385	CB	LEU	B	727	30.055	30.948	29.985	1.00	29.25
30	2386	CG	LEU	B	727	28.749	30.917	30.766	1.00	39.65
	2387	CD1	LEU	B	727	27.887	32.091	30.358	1.00	38.17
	2388	CD2	LEU	B	727	28.028	29.603	30.492	1.00	38.71
35	2389	N	SER	B	728	33.159	30.701	29.407	1.00	22.52
	2390	CA	SER	B	728	34.247	30.790	28.442	1.00	25.41
	2391	C	SER	B	728	35.132	29.550	28.475	1.00	22.52
40	2392	O	SER	B	728	35.628	29.129	27.438	1.00	19.75
	2393	CB	SER	B	728	35.088	32.069	28.644	1.00	28.09
	2394	OG	SER	B	728	35.801	32.055	29.860	1.00	44.44
45	2395	N	VAL	B	729	35.337	28.982	29.665	1.00	20.70
	2396	CA	VAL	B	729	36.107	27.739	29.814	1.00	20.20
	2397	C	VAL	B	729	35.413	26.610	29.050	1.00	16.88
50	2398	O	VAL	B	729	36.066	25.812	28.386	1.00	19.20
	2399	CB	VAL	B	729	36.215	27.328	31.297	1.00	20.97
	2400	CG1	VAL	B	729	36.711	25.900	31.440	1.00	22.68
55	2401	CG2	VAL	B	729	37.177	28.284	32.010	1.00	26.21
	2402	N	VAL	B	730	34.092	26.523	29.154	1.00	18.77
	2403	CA	VAL	B	730	33.400	25.461	28.434	1.00	20.28
55	2404	C	VAL	B	730	33.605	25.648	26.931	1.00	18.42
	2405	O	VAL	B	730	33.973	24.706	26.239	1.00	21.52
	2406	CB	VAL	B	730	31.901	25.420	28.772	1.00	21.49
	2407	CG1	VAL	B	730	31.228	24.300	27.947	1.00	25.40

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2408	CG2	VAL	B	730	31.721	25.149	30.252	1.00	24.07
2409	N	LYS	B	731	33.397	26.870	26.442	1.00	22.29
2410	CA	LYS	B	731	33.591	27.195	25.024	1.00	22.57
2411 1	C	LYS	B	731	35.017	26.824	24.589	1.00	22.82
2412	O	LYS	B	731	35.231	26.168	23.567	1.00	20.83
2413	CB	LYS	B	731	33.358	28.695	24.816	1.00	27.41
2414	CG	LYS	B	731	33.541	29.215	23.377	1.00	33.69
2415	CD	LYS	B	731	32.513	28.628	22.415	1.00	42.24
2416	CE	LYS	B	731	32.628	29.239	21.010	1.00	43.85
2417	NZ	LYS	B	731	33.961	29.015	20.381	1.00	43.69
2418	N	TRP	B	732	35.999	27.266	25.372	1.00	19.99
2419	CA	TRP	B	732	37.401	26.981	25.106	1.00	20.03
2420	C	TRP	B	732	37.668	25.471	25.013	1.00	22.42
2421	O	TRP	B	732	38.343	25.003	24.098	1.00	21.10
2422	CB	TRP	B	732	38.242	27.603	26.233	1.00	21.24
2423	CG	TRP	B	732	39.702	27.242	26.283	1.00	23.70
2424	CD1	TRP	B	732	40.696	27.670	25.444	1.00	24.42
2425	CD2	TRP	B	732	40.336	26.404	27.260	1.00	25.32
2426	NE1	TRP	B	732	41.906	27.154	25.843	1.00	24.62
2427	CE2	TRP	B	732	41.715	26.373	26.954	1.00	23.58
2428	CE3	TRP	B	732	39.869	25.677	28.368	1.00	23.75
2429	CZ2	TRP	B	732	42.640	25.640	27.716	1.00	21.37
2430	CZ3	TRP	B	732	40.794	24.946	29.131	1.00	25.72
2431	CH2	TRP	B	732	42.160	24.935	28.797	1.00	25.44
2432	N	SER	B	733	37.122	24.710	25.953	1.00	20.29
2433	CA	SER	B	733	37.354	23.263	25.985	1.00	17.86
2434	C	SER	B	733	36.817	22.570	24.725	1.00	17.55
2435	O	SER	B	733	37.352	21.539	24.298	1.00	19.01
2436	CB	SER	B	733	36.718	22.637	27.246	1.00	21.68
2437	OG	SER	B	733	35.305	22.650	27.205	1.00	23.79
2438	N	LYS	B	734	35.777	23.160	24.133	1.00	21.12
2439	CA	LYS	B	734	35.179	22.608	22.917	1.00	19.68
2440	C	LYS	B	734	36.090	22.818	21.712	1.00	20.73
2441	O	LYS	B	734	35.969	22.107	20.715	1.00	22.12
2442	CB	LYS	B	734	33.825	23.256	22.623	1.00	24.55
2443	CG	LYS	B	734	32.716	22.963	23.615	1.00	32.49
2444	CD	LYS	B	734	31.394	23.451	23.040	1.00	42.26

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2445	CE	LYS	B	734	30.205	23.137	23.936	1.00	40.61
	2446	NZ	LYS	B	734	30.231	23.960	25.168	1.00	48.42
	2447	N	SER	B	735	37.000	23.788	21.806	1.00	19.46
10	2448	CA	SER	B	735	37.937	24.086	20.721	1.00	23.70
	2449	C	SER	B	735	39.327	23.512	21.008	1.00	22.09
	2450	O	SER	B	735	40.174	23.495	20.142	1.00	24.41
15	2451	CB	SER	B	735	38.086	25.597	20.521	1.00	27.76
	2452	OG	SER	B	735	36.848	26.243	20.279	1.00	31.96
	2453	N	LEU	B	736	39.535	23.048	22.232	1.00	23.63
20	2454	CA	LEU	B	736	40.817	22.494	22.665	1.00	20.47
	2455	C	LEU	B	736	41.113	21.140	22.021	1.00	21.67
	2456	O	LEU	B	736	40.393	20.170	22.231	1.00	22.30
25	2457	CB	LEU	B	736	40.801	22.353	24.184	1.00	22.13
	2458	CG	LEU	B	736	42.046	21.828	24.877	1.00	25.58
	2459	CD1	LEU	B	736	43.226	22.778	24.641	1.00	24.77
30	2460	CD2	LEU	B	736	41.735	21.702	26.376	1.00	24.96
	2461	N	PRO	B	737	42.192	21.058	21.227	1.00	24.15
	2462	CA	PRO	B	737	42.559	19.806	20.561	1.00	27.85
35	2463	C	PRO	B	737	42.607	18.605	21.497	1.00	29.75
	2464	O	PRO	B	737	43.323	18.596	22.514	1.00	25.17
	2465	CB	PRO	B	737	43.923	20.136	19.967	1.00	31.60
40	2466	CG	PRO	B	737	43.757	21.565	19.610	1.00	24.35
	2467	CD	PRO	B	737	43.177	22.102	20.900	1.00	27.34
	2468	N	GLY	B	738	41.809	17.605	21.149	1.00	25.39
45	2469	CA	GLY	B	738	41.747	16.381	21.916	1.00	26.62
	2470	C	GLY	B	738	40.624	16.272	22.931	1.00	23.45
	2471	O	GLY	B	738	40.090	15.194	23.141	1.00	26.46
50	2472	N	PHE	B	739	40.229	17.383	23.539	1.00	24.87
	2473	CA	PHE	B	739	39.218	17.335	24.585	1.00	19.47
	2474	C	PHE	B	739	37.860	16.782	24.178	1.00	25.30
55	2475	O	PHE	B	739	37.301	15.944	24.874	1.00	21.67
	2476	CB	PHE	B	739	39.015	18.714	25.175	1.00	17.19
	2477	CG	PHE	B	739	38.439	18.692	26.559	1.00	23.41
	2478	CD1	PHE	B	739	39.182	18.176	27.617	1.00	28.09
	2479	CD2	PHE	B	739	37.178	19.218	26.814	1.00	25.22
	2480	CE1	PHE	B	739	38.674	18.200	28.907	1.00	26.53
	2481	CE2	PHE	B	739	36.662	19.245	28.109	1.00	23.43

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	2482	CZ	PHE	B	739	37.413	18.738	29.152	1.00	27.21
	2483	N	ARG	B	740	37.329	17.252	23.055	1.00	23.16
	2484	CA	ARG	B	740	36.008	16.801	22.599	1.00	24.65
10	2485	C	ARG	B	740	35.942	15.298	22.331	1.00	26.61
	2486	O	ARG	B	740	34.854	14.739	22.213	1.00	32.12
	2487	CB	ARG	B	740	35.607	17.534	21.318	1.00	22.44
15	2488	CG	ARG	B	740	36.578	17.308	20.173	1.00	25.67
	2489	CD	ARG	B	740	36.001	17.852	18.873	1.00	25.78
	2490	NE	ARG	B	740	36.906	17.610	17.757	1.00	22.52
20	2491	CZ	ARG	B	740	36.605	17.907	16.497	1.00	27.51
	2492	NH1	ARG	B	740	35.428	18.444	16.212	1.00	25.90
	2493	NH2	ARG	B	740	37.473	17.658	15.532	1.00	24.02
25	2494	N	ASN	B	741	37.102	14.654	22.236	1.00	24.93
	2495	CA	ASN	B	741	37.147	13.229	21.956	1.00	27.05
	2496	C	ASN	B	741	37.072	12.358	23.206	1.00	28.80
30	2497	O	ASN	B	741	37.020	11.136	23.109	1.00	27.35
	2498	CB	ASN	B	741	38.392	12.925	21.134	1.00	29.54
	2499	CG	ASN	B	741	38.408	13.689	19.821	1.00	28.39
35	2500	OD1	ASN	B	741	39.465	14.059	19.312	1.00	29.43
	2501	ND2	ASN	B	741	37.226	13.916	19.263	1.00	25.86
	2502	N	LEU	B	742	37.069	12.989	24.379	1.00	27.36
40	2503	CA	LEU	B	742	36.922	12.258	25.632	1.00	26.94
	2504	C	LEU	B	742	35.414	12.108	25.808	1.00	25.47
	2505	O	LEU	B	742	34.648	12.905	25.273	1.00	27.23
45	2506	CB	LEU	B	742	37.491	13.064	26.813	1.00	23.76
	2507	CG	LEU	B	742	38.995	13.350	26.739	1.00	25.50
	2508	CD1	LEU	B	742	39.449	14.126	27.976	1.00	29.97
50	2509	CD2	LEU	B	742	39.751	12.040	26.658	1.00	28.27
	2510	N	HIS	B	743	34.987	11.088	26.542	1.00	22.87
	2511	CA	HIS	B	743	33.565	10.873	26.786	1.00	26.83
55	2512	C	HIS	B	743	33.009	12.167	27.392	1.00	26.76
	2513	O	HIS	B	743	33.701	12.835	28.171	1.00	24.67
	2514	CB	HIS	B	743	33.402	9.691	27.741	1.00	30.89
55	2515	CG	HIS	B	743	31.996	9.201	27.874	1.00	35.28
	2516	ND1	HIS	B	743	31.008	9.918	28.515	1.00	36.31
	2517	CD2	HIS	B	743	31.410	8.057	27.443	1.00	38.01
	2518	CE1	HIS	B	743	29.875	9.238	28.473	1.00	41.45

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2519	NE2	HIS	B	743	30.093	8.105	27.828	1.00	34.92
	2520	N	ILE	B	744	31.784	12.541	27.018	1.00	25.83
	2521	CA	ILE	B	744	31.172	13.769	27.536	1.00	28.41
10	2522	C	ILE	B	744	31.205	13.806	29.068	1.00	27.71
	2523	O	ILE	B	744	31.410	14.868	29.669	1.00	25.71
	2524	CB	ILE	B	744	29.695	13.919	27.053	1.00	29.59
15	2525	CG1	ILE	B	744	29.082	15.205	27.610	1.00	37.61
	2526	CG2	ILE	B	744	28.869	12.710	27.499	1.00	32.16
	2527	CD1	ILE	B	744	29.747	16.482	27.116	1.00	40.77
20	2528	N	ASP	B	745	31.006	12.658	29.711	1.00	25.28
	2529	CA	ASP	B	745	31.037	12.657	31.168	1.00	26.77
	2530	C	ASP	B	745	32.424	13.001	31.733	1.00	29.51
25	2531	O	ASP	B	745	32.524	13.657	32.780	1.00	24.05
	2532	CB	ASP	B	745	30.544	11.318	31.722	1.00	35.05
	2533	CG	ASP	B	745	29.068	11.075	31.418	1.00	36.78
30	2534	OD1	ASP	B	745	28.266	12.015	31.582	1.00	47.93
	2535	OD2	ASP	B	745	28.707	9.946	31.033	1.00	51.31
	2536	N	ASP	B	746	33.492	12.557	31.062	1.00	24.59
35	2537	CA	ASP	B	746	34.836	12.900	31.536	1.00	25.82
	2538	C	ASP	B	746	35.098	14.400	31.324	1.00	24.98
	2539	O	ASP	B	746	35.762	15.049	32.130	1.00	23.59
40	2540	CB	ASP	B	746	35.935	12.125	30.804	1.00	27.37
	2541	CG	ASP	B	746	35.774	10.616	30.908	1.00	35.48
	2542	OD1	ASP	B	746	35.307	10.109	31.957	1.00	33.88
45	2543	OD2	ASP	B	746	36.155	9.937	29.933	1.00	34.19
	2544	N	GLN	B	747	34.597	14.948	30.222	1.00	23.17
	2545	CA	GLN	B	747	34.794	16.367	29.946	1.00	23.00
50	2546	C	GLN	B	747	34.183	17.197	31.056	1.00	19.52
	2547	O	GLN	B	747	34.805	18.141	31.563	1.00	21.92
	2548	CB	GLN	B	747	34.139	16.761	28.617	1.00	20.19
55	2549	CG	GLN	B	747	34.774	16.122	27.398	1.00	18.51
	2550	CD	GLN	B	747	34.103	16.560	26.104	1.00	29.12
	2551	OE1	GLN	B	747	33.915	17.747	25.876	1.00	22.13
55	2552	NE2	GLN	B	747	33.760	15.601	25.243	1.00	22.48
	2553	N	ILE	B	748	32.948	16.855	31.415	1.00	20.67
	2554	CA	ILE	B	748	32.247	17.575	32.454	1.00	24.05
	2555	C	ILE	B	748	32.978	17.422	33.766	1.00	23.11

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2556	O	ILE	B	748	33.196	18.404	34.471	1.00	20.45
	2557	CB	ILE	B	748	30.802	17.085	32.581	1.00	24.48
	2558	CG1	ILE	B	748	30.032	17.501	31.328	1.00	28.95
10	2559	CG2	ILE	B	748	30.146	17.674	33.830	1.00	28.57
	2560	CD1	ILE	B	748	28.623	16.921	31.244	1.00	37.34
	2561	N	THR	B	749	33.388	16.200	34.076	1.00	19.37
15	2562	CA	THR	B	749	34.108	15.961	35.320	1.00	22.97
	2563	C	THR	B	749	35.404	16.768	35.376	1.00	19.50
	2564	O	THR	B	749	35.698	17.391	36.390	1.00	20.73
20	2565	CB	THR	B	749	34.439	14.464	35.492	1.00	27.90
	2566	OG1	THR	B	749	33.218	13.724	35.603	1.00	30.62
	2567	CG2	THR	B	749	35.269	14.238	36.742	1.00	31.03
25	2568	N	LEU	B	750	36.170	16.780	34.286	1.00	19.81
	2569	CA	LEU	B	750	37.433	17.526	34.295	1.00	20.44
	2570	C	LEU	B	750	37.232	19.026	34.495	1.00	23.24
30	2571	O	LEU	B	750	38.015	19.676	35.186	1.00	17.97
	2572	CB	LEU	B	750	38.223	17.259	33.002	1.00	23.58
	2573	CG	LEU	B	750	38.682	15.795	32.882	1.00	22.85
35	2574	CD1	LEU	B	750	39.218	15.509	31.477	1.00	22.39
	2575	CD2	LEU	B	750	39.776	15.524	33.922	1.00	26.05
	2576	N	ILE	B	751	36.193	19.587	33.881	1.00	16.58
40	2577	CA	ILE	B	751	35.930	21.000	34.061	1.00	19.30
	2578	C	ILE	B	751	35.486	21.264	35.503	1.00	19.20
	2579	O	ILE	B	751	35.894	22.258	36.112	1.00	20.53
45	2580	CB	ILE	B	751	34.862	21.477	33.064	1.00	19.73
	2581	CG1	ILE	B	751	35.477	21.535	31.655	1.00	17.39
	2582	CG2	ILE	B	751	34.333	22.842	33.474	1.00	19.69
50	2583	CD1	ILE	B	751	34.453	21.888	30.553	1.00	25.86
	2584	N	GLN	B	752	34.649	20.377	36.039	1.00	17.90
	2585	CA	GLN	B	752	34.167	20.524	37.407	1.00	19.84
55	2586	C	GLN	B	752	35.290	20.395	38.424	1.00	22.37
	2587	O	GLN	B	752	35.241	21.000	39.485	1.00	20.97
	2588	CB	GLN	B	752	33.067	19.502	37.702	1.00	23.55
55	2589	CG	GLN	B	752	31.771	19.857	36.983	1.00	23.27
	2590	CD	GLN	B	752	30.646	18.872	37.223	1.00	27.86
	2591	OE1	GLN	B	752	29.481	19.154	36.920	1.00	30.08
	2592	NE2	GLN	B	752	30.980	17.714	37.735	1.00	21.11

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2593	N	TYR	B	753	36.299	19.588	38.102	1.00	16.66
	2594	CA	TYR	B	753	37.444	19.437	39.013	1.00	21.25
	2595	C	TYR	B	753	38.451	20.586	38.939	1.00	21.49
10	2596	O	TYR	B	753	39.049	20.985	39.945	1.00	28.69
	2597	CB	TYR	B	753	38.256	18.186	38.682	1.00	19.38
	2598	CG	TYR	B	753	37.659	16.849	39.059	1.00	26.62
15	2599	CD1	TYR	B	753	36.491	16.747	39.813	1.00	24.99
	2600	CD2	TYR	B	753	38.323	15.668	38.710	1.00	27.30
	2601	CE1	TYR	B	753	36.007	15.502	40.215	1.00	28.65
20	2602	CE2	TYR	B	753	37.850	14.432	39.106	1.00	26.34
	2603	CZ	TYR	B	753	36.707	14.347	39.853	1.00	29.07
	2604	OH	TYR	B	753	36.282	13.103	40.254	1.00	34.63
25	2605	N	SER	B	754	38.639	21.126	37.744	1.00	20.94
	2606	CA	SER	B	754	39.679	22.122	37.540	1.00	20.30
	2607	C	SER	B	754	39.318	23.587	37.387	1.00	20.01
30	2608	O	SER	B	754	40.218	24.404	37.314	1.00	20.79
	2609	CB	SER	B	754	40.476	21.734	36.297	1.00	26.89
	2610	OG	SER	B	754	39.650	21.929	35.155	1.00	24.56
35	2611	N	TRP	B	755	38.040	23.943	37.347	1.00	18.81
	2612	CA	TRP	B	755	37.710	25.352	37.136	1.00	21.09
	2613	C	TRP	B	755	38.414	26.366	38.060	1.00	22.06
40	2614	O	TRP	B	755	38.864	27.419	37.598	1.00	21.85
	2615	CB	TRP	B	755	36.188	25.585	37.199	1.00	19.53
	2616	CG	TRP	B	755	35.576	25.368	38.537	1.00	19.91
45	2617	CD1	TRP	B	755	35.105	24.196	39.045	1.00	22.90
	2618	CD2	TRP	B	755	35.393	26.354	39.557	1.00	24.20
	2619	NE1	TRP	B	755	34.636	24.389	40.323	1.00	25.70
50	2620	CE2	TRP	B	755	34.804	25.707	40.661	1.00	19.09
	2621	CE3	TRP	B	755	35.672	27.728	39.643	1.00	23.21
	2622	CZ2	TRP	B	755	34.486	26.379	41.842	1.00	22.66
55	2623	CZ3	TRP	B	755	35.356	28.394	40.811	1.00	25.02
	2624	CH2	TRP	B	755	34.767	27.720	41.900	1.00	26.92
	2625	N	MET	B	756	38.512	26.084	39.353	1.00	20.39
55	2626	CA	MET	B	756	39.169	27.042	40.249	1.00	22.21
	2627	C	MET	B	756	40.641	27.207	39.885	1.00	18.94
	2628	O	MET	B	756	41.183	28.334	39.891	1.00	21.30
	2629	CB	MET	B	756	39.051	26.592	41.720	1.00	24.34

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2630	CG	MET	B	756	39.665	27.592	42.706	1.00	22.35
	2631	SD	MET	B	756	38.654	29.079	42.939	1.00	27.19
	2632	CE	MET	B	756	37.316	28.325	43.999	1.00	23.83
10	2633	N	SER	B	757	41.289	26.098	39.556	1.00	20.58
	2634	CA	SER	B	757	42.700	26.133	39.208	1.00	21.19
	2635	C	SER	B	757	42.875	26.932	37.917	1.00	20.60
15	2636	O	SER	B	757	43.734	27.793	37.820	1.00	19.30
	2637	CB	SER	B	757	43.254	24.702	39.054	1.00	25.76
	2638	OG	SER	B	757	42.837	24.114	37.832	1.00	34.55
20	2639	N	LEU	B	758	42.050	26.665	36.915	1.00	18.54
	2640	CA	LEU	B	758	42.149	27.419	35.678	1.00	20.03
	2641	C	LEU	B	758	41.929	28.915	35.894	1.00	19.30
25	2642	O	LEU	B	758	42.652	29.749	35.323	1.00	21.43
	2643	CB	LEU	B	758	41.122	26.896	34.667	1.00	20.21
	2644	CG	LEU	B	758	41.373	25.461	34.198	1.00	25.47
30	2645	CD1	LEU	B	758	40.154	24.953	33.419	1.00	26.99
	2646	CD2	LEU	B	758	42.649	25.424	33.351	1.00	22.02
	2647	N	MET	B	759	40.949	29.282	36.721	1.00	19.96
35	2648	CA	MET	B	759	40.679	30.702	36.916	1.00	17.34
	2649	C	MET	B	759	41.713	31.441	37.742	1.00	19.85
	2650	O	MET	B	759	42.016	32.600	37.455	1.00	21.26
40	2651	CB	MET	B	759	39.268	30.914	37.491	1.00	21.30
	2652	CG	MET	B	759	38.202	30.434	36.522	1.00	25.18
	2653	SD	MET	B	759	36.495	30.703	37.019	1.00	32.88
45	2654	CE	MET	B	759	35.638	29.677	35.765	1.00	35.46
	2655	N	VAL	B	760	42.282	30.788	38.748	1.00	19.44
	2656	CA	VAL	B	760	43.288	31.476	39.548	1.00	22.37
50	2657	C	VAL	B	760	44.582	31.585	38.723	1.00	23.17
	2658	O	VAL	B	760	45.346	32.547	38.842	1.00	22.82
	2659	CB	VAL	B	760	43.511	30.753	40.921	1.00	22.03
55	2660	CG1	VAL	B	760	44.296	29.450	40.762	1.00	22.24
	2661	CG2	VAL	B	760	44.161	31.725	41.908	1.00	26.70
	2662	N	PHE	B	761	44.810	30.611	37.847	1.00	23.09
55	2663	CA	PHE	B	761	45.989	30.643	36.989	1.00	24.16
	2664	C	PHE	B	761	45.832	31.784	35.978	1.00	23.45
	2665	O	PHE	B	761	46.794	32.493	35.674	1.00	24.87
	2666	CB	PHE	B	761	46.128	29.298	36.266	1.00	25.81

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2667	CG	PHE	B	761	47.512	29.020	35.741	1.00	25.64
	2668	CD1	PHE	B	761	48.586	28.889	36.616	1.00	25.18
	2669	CD2	PHE	B	761	47.719	28.794	34.383	1.00	19.58
10	2670	CE1	PHE	B	761	49.836	28.528	36.135	1.00	27.13
	2671	CE2	PHE	B	761	48.964	28.430	33.895	1.00	25.89
	2672	CZ	PHE	B	761	50.026	28.294	34.770	1.00	26.79
15	2673	N	GLY	B	762	44.619	31.932	35.445	1.00	26.41
	2674	CA	GLY	B	762	44.315	32.988	34.493	1.00	22.56
	2675	C	GLY	B	762	44.459	34.341	35.170	1.00	24.22
20	2676	O	GLY	B	762	45.005	35.281	34.588	1.00	22.86
	2677	N	LEU	B	763	43.966	34.441	36.406	1.00	22.38
	2678	CA	LEU	B	763	44.083	35.674	37.186	1.00	20.84
25	2679	C	LEU	B	763	45.567	36.032	37.319	1.00	23.50
	2680	O	LEU	B	763	45.961	37.202	37.183	1.00	23.47
	2681	CB	LEU	B	763	43.490	35.476	38.586	1.00	25.56
30	2682	CG	LEU	B	763	43.743	36.570	39.641	1.00	19.73
	2683	CD1	LEU	B	763	43.178	37.897	39.172	1.00	20.52
	2684	CD2	LEU	B	763	43.081	36.166	40.948	1.00	21.82
35	2685	N	GLY	B	764	46.379	35.015	37.588	1.00	23.30
	2686	CA	GLY	B	764	47.805	35.230	37.747	1.00	26.93
	2687	C	GLY	B	764	48.398	35.805	36.481	1.00	28.28
40	2688	O	GLY	B	764	49.167	36.768	36.511	1.00	31.36
	2689	N	TRP	B	765	48.025	35.220	35.351	1.00	23.45
	2690	CA	TRP	B	765	48.539	35.681	34.073	1.00	27.13
45	2691	C	TRP	B	765	48.133	37.117	33.746	1.00	26.40
	2692	O	TRP	B	765	48.970	37.924	33.333	1.00	29.82
	2693	CB	TRP	B	765	48.091	34.726	32.961	1.00	26.89
50	2694	CG	TRP	B	765	48.662	35.089	31.648	1.00	26.96
	2695	CD1	TRP	B	765	48.053	35.775	30.641	1.00	29.28
	2696	CD2	TRP	B	765	50.019	34.893	31.241	1.00	26.36
55	2697	NE1	TRP	B	765	48.951	36.022	29.630	1.00	29.91
	2698	CE2	TRP	B	765	50.167	35.493	29.975	1.00	31.07
	2699	CE3	TRP	B	765	51.127	34.270	31.832	1.00	29.13
55	2700	CZ2	TRP	B	765	51.388	35.489	29.279	1.00	33.25
	2701	CZ3	TRP	B	765	52.342	34.264	31.140	1.00	32.77
	2702	CH2	TRP	B	765	52.456	34.868	29.881	1.00	26.10
	2703	N	ARG	B	766	46.855	37.451	33.924	1.00	25.83

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	2704	CA	ARG	B	766	46.406	38.808	33.639	1.00	24.82
	2705	C	ARG	B	766	47.084	39.831	34.538	1.00	24.76
	2706	O	ARG	B	766	47.389	40.943	34.104	1.00	28.34
10	2707	CB	ARG	B	766	44.883	38.939	33.808	1.00	26.93
	2708	CG	ARG	B	766	44.047	38.200	32.774	1.00	24.24
	2709	CD	ARG	B	766	42.589	38.568	32.948	1.00	26.44
15	2710	NE	ARG	B	766	42.078	38.160	34.256	1.00	26.20
	2711	CZ	ARG	B	766	41.655	36.932	34.559	1.00	23.20
	2712	NH1	ARG	B	766	41.673	35.975	33.656	1.00	26.38
20	2713	NH2	ARG	B	766	41.210	36.665	35.784	1.00	23.30
	2714	N	SER	B	767	47.322	39.465	35.793	1.00	21.83
	2715	CA	SER	B	767	47.954	40.405	36.721	1.00	24.98
25	2716	C	SER	B	767	49.388	40.617	36.273	1.00	26.41
	2717	O	SER	B	767	49.878	41.740	36.209	1.00	26.61
	2718	CB	SER	B	767	47.961	39.857	38.147	1.00	24.94
30	2719	OG	SER	B	767	46.653	39.669	38.646	1.00	30.28
	2720	N	TYR	B	768	50.050	39.512	35.967	1.00	29.18
	2721	CA	TYR	B	768	51.436	39.532	35.514	1.00	30.71
35	2722	C	TYR	B	768	51.631	40.356	34.241	1.00	34.29
	2723	O	TYR	B	768	52.572	41.143	34.137	1.00	37.28
	2724	CB	TYR	B	768	51.890	38.082	35.319	1.00	31.45
40	2725	CG	TYR	B	768	53.208	37.878	34.597	1.00	36.24
	2726	CD1	TYR	B	768	54.365	38.560	34.984	1.00	38.98
	2727	CD2	TYR	B	768	53.308	36.950	33.560	1.00	38.42
45	2728	CE1	TYR	B	768	55.590	38.317	34.356	1.00	40.04
	2729	CE2	TYR	B	768	54.525	36.700	32.929	1.00	40.42
	2730	CZ	TYR	B	768	55.661	37.386	33.331	1.00	43.23
50	2731	OH	TYR	B	768	56.865	37.125	32.706	1.00	51.72
	2732	N	LYS	B	769	50.707	40.223	33.300	1.00	33.52
	2733	CA	LYS	B	769	50.828	40.907	32.018	1.00	37.03
55	2734	C	LYS	B	769	50.290	42.338	31.934	1.00	36.01
	2735	O	LYS	B	769	50.755	43.115	31.103	1.00	33.96
	2736	CB	LYS	B	769	50.172	40.031	30.943	1.00	41.58
	2737	CG	LYS	B	769	50.422	40.435	29.497	1.00	50.59
	2738	CD	LYS	B	769	49.872	39.351	28.577	1.00	52.94
	2739	CE	LYS	B	769	50.140	39.630	27.113	1.00	55.40
	2740	NZ	LYS	B	769	49.610	38.525	26.263	1.00	56.70

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2741	N	HIS	B	770	49.329	42.700	32.780	1.00	35.24
	2742	CA	HIS	B	770	48.758	44.047	32.723	1.00	34.60
	2743	C	HIS	B	770	49.204	45.022	33.790	1.00	36.43
10	2744	O	HIS	B	770	49.272	46.229	33.541	1.00	34.37
	2745	CB	HIS	B	770	47.236	43.983	32.747	1.00	35.70
	2746	CG	HIS	B	770	46.649	43.272	31.573	1.00	46.81
15	2747	ND1	HIS	B	770	46.827	43.706	30.277	1.00	50.52
	2748	CD2	HIS	B	770	45.892	42.152	31.496	1.00	49.20
	2749	CE1	HIS	B	770	46.205	42.883	29.452	1.00	49.27
20	2750	NE2	HIS	B	770	45.630	41.932	30.165	1.00	51.77
	2751	N	VAL	B	771	49.487	44.520	34.985	1.00	33.76
	2752	CA	VAL	B	771	49.907	45.409	36.054	1.00	32.20
25	2753	C	VAL	B	771	51.229	44.988	36.679	1.00	30.98
	2754	O	VAL	B	771	51.479	45.235	37.852	1.00	34.33
	2755	CB	VAL	B	771	48.795	45.520	37.136	1.00	34.95
30	2756	CG1	VAL	B	771	47.603	46.297	36.576	1.00	33.50
	2757	CG2	VAL	B	771	48.332	44.140	37.557	1.00	29.74
	2758	N	SER	B	772	52.075	44.350	35.878	1.00	30.62
35	2759	CA	SER	B	772	53.386	43.907	36.338	1.00	31.95
	2760	C	SER	B	772	53.284	43.015	37.561	1.00	33.92
	2761	O	SER	B	772	54.226	42.930	38.350	1.00	30.00
40	2762	CB	SER	B	772	54.256	45.117	36.674	1.00	34.85
	2763	OG	SER	B	772	54.357	45.981	35.558	1.00	43.83
	2764	N	GLY	B	773	52.128	42.371	37.724	1.00	28.37
45	2765	CA	GLY	B	773	51.917	41.473	38.844	1.00	29.00
	2766	C	GLY	B	773	51.706	42.154	40.186	1.00	26.33
	2767	O	GLY	B	773	51.644	41.482	41.224	1.00	26.94
50	2768	N	GLN	B	774	51.554	43.474	40.177	1.00	24.89
	2769	CA	GLN	B	774	51.411	44.204	41.429	1.00	26.11
	2770	C	GLN	B	774	49.994	44.597	41.871	1.00	28.67
55	2771	O	GLN	B	774	49.818	45.376	42.811	1.00	27.16
	2772	CB	GLN	B	774	52.345	45.425	41.417	1.00	25.33
	2773	CG	GLN	B	774	53.803	45.022	41.149	1.00	29.08
55	2774	CD	GLN	B	774	54.233	43.816	41.973	1.00	27.66
	2775	OE1	GLN	B	774	54.227	43.848	43.216	1.00	30.12
	2776	NE2	GLN	B	774	54.600	42.738	41.289	1.00	30.15
	2777	N	MET	B	775	48.993	44.041	41.196	1.00	24.77

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2778	CA	MET	B	775	47.589	44.238	41.560	1.00	26.82
2779	C	MET	B	775	46.920	42.961	41.091	1.00	24.83
2780	O	MET	B	775	47.494	42.244	40.288	1.00	26.99
2781	CB	MET	B	775	46.952	45.419	40.827	1.00	28.09
2782	CG	MET	B	775	47.653	46.741	41.024	1.00	26.44
2783	SD	MET	B	775	46.706	48.019	40.194	1.00	37.11
2784	CE	MET	B	775	47.958	49.275	39.887	1.00	41.20
2785	N	LEU	B	776	45.739	42.655	41.611	1.00	26.95
2786	CA	LEU	B	776	45.017	41.454	41.176	1.00	23.64
2787	C	LEU	B	776	44.072	41.936	40.097	1.00	25.94
2788	O	LEU	B	776	43.125	42.672	40.372	1.00	26.27
2789	CB	LEU	B	776	44.235	40.826	42.330	1.00	26.64
2790	CG	LEU	B	776	45.070	40.094	43.390	1.00	27.80
2791	CD1	LEU	B	776	44.161	39.532	44.462	1.00	26.56
2792	CD2	LEU	B	776	45.855	38.956	42.735	1.00	29.50
2793	N	TYR	B	777	44.357	41.521	38.868	1.00	23.88
2794	CA	TYR	B	777	43.590	41.934	37.705	1.00	23.44
2795	C	TYR	B	777	42.525	40.892	37.399	1.00	25.02
2796	O	TYR	B	777	42.665	40.086	36.477	1.00	22.33
2797	CB	TYR	B	777	44.565	42.113	36.533	1.00	27.34
2798	CG	TYR	B	777	44.011	42.846	35.342	1.00	29.61
2799	CD1	TYR	B	777	43.122	42.230	34.463	1.00	32.26
2800	CD2	TYR	B	777	44.397	44.155	35.078	1.00	30.45
2801	CE1	TYR	B	777	42.644	42.899	33.350	1.00	32.66
2802	CE2	TYR	B	777	43.926	44.834	33.971	1.00	33.13
2803	CZ	TYR	B	777	43.054	44.205	33.108	1.00	34.40
2804	OH	TYR	B	777	42.624	44.877	31.982	1.00	34.07
2805	N	PHE	B	778	41.463	40.899	38.204	1.00	22.02
2806	CA	PHE	B	778	40.359	39.952	38.004	1.00	24.28
2807	C	PHE	B	778	39.700	40.235	36.663	1.00	24.40
2808	O	PHE	B	778	39.355	39.313	35.916	1.00	23.54
2809	CB	PHE	B	778	39.329	40.097	39.126	1.00	20.00
2810	CG	PHE	B	778	39.805	39.594	40.444	1.00	21.83
2811	CD1	PHE	B	778	39.841	38.227	40.709	1.00	21.24
2812	CD2	PHE	B	778	40.238	40.482	41.426	1.00	25.82
2813	CE1	PHE	B	778	40.299	37.762	41.930	1.00	24.17
2814	CE2	PHE	B	778	40.702	40.013	42.656	1.00	21.13

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2815	CZ	PHE	B	778	40.729	38.650	42.901	1.00	21.77
2816	N	ALA	B	779	39.530	41.522	36.367	1.00	22.16
2817	CA	ALA	B	779	38.930	41.976	35.113	1.00	24.84
2818	C	ALA	B	779	39.289	43.453	34.917	1.00	25.04
2819	O	ALA	B	779	39.724	44.114	35.850	1.00	25.47
2820	CB	ALA	B	779	37.407	41.814	35.155	1.00	20.33
2821	N	PRO	B	780	39.075	43.995	33.708	1.00	29.20
2822	CA	PRO	B	780	39.412	45.403	33.488	1.00	31.77
2823	C	PRO	B	780	38.656	46.367	34.407	1.00	33.65
2824	O	PRO	B	780	39.149	47.463	34.704	1.00	31.21
2825	CB	PRO	B	780	39.066	45.603	32.004	1.00	33.06
2826	CG	PRO	B	780	39.260	44.203	31.433	1.00	37.79
2827	CD	PRO	B	780	38.515	43.414	32.480	1.00	28.89
2828	N	ASP	B	781	37.465	45.951	34.851	1.00	30.03
2829	CA	ASP	B	781	36.603	46.758	35.719	1.00	27.54
2830	C	ASP	B	781	36.606	46.262	37.171	1.00	30.56
2831	O	ASP	B	781	35.774	46.680	37.987	1.00	30.31
2832	CB	ASP	B	781	35.163	46.739	35.172	1.00	30.77
2833	CG	ASP	B	781	34.536	45.344	35.210	1.00	32.93
2834	OD1	ASP	B	781	35.251	44.350	34.942	1.00	30.51
2835	OD2	ASP	B	781	33.317	45.240	35.482	1.00	38.32
2836	N	LEU	B	782	37.539	45.368	37.485	1.00	28.57
2837	CA	LEU	B	782	37.667	44.820	38.833	1.00	27.89
2838	C	LEU	B	782	39.135	44.522	39.090	1.00	27.07
2839	O	LEU	B	782	39.611	43.382	38.993	1.00	25.66
2840	CB	LEU	B	782	36.808	43.555	38.996	1.00	23.48
2841	CG	LEU	B	782	36.673	43.026	40.431	1.00	27.04
2842	CD1	LEU	B	782	36.229	44.163	41.340	1.00	30.90
2843	CD2	LEU	B	782	35.666	41.850	40.492	1.00	26.37
2844	N	ILE	B	783	39.860	45.584	39.399	1.00	26.64
2845	CA	ILE	B	783	41.279	45.491	39.675	1.00	28.26
2846	C	ILE	B	783	41.460	45.862	41.126	1.00	25.73
2847	O	ILE	B	783	40.948	46.879	41.587	1.00	29.13
2848	CB	ILE	B	783	42.070	46.471	38.778	1.00	28.66
2849	CG1	ILE	B	783	41.847	46.101	37.314	1.00	28.24
2850	CG2	ILE	B	783	43.552	46.422	39.108	1.00	30.46
2851	CD1	ILE	B	783	42.448	47.084	36.325	1.00	33.70

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
2852	N	LEU	B	784	42.175	45.022	41.855	1.00	30.10
2853	CA	LEU	B	784	42.400	45.278	43.263	1.00	27.98
2854	C	LEU	B	784	43.870	45.525	43.576	1.00	26.93
2855	O	LEU	B	784	44.663	44.587	43.507	1.00	24.54
2856	CB	LEU	B	784	41.969	44.081	44.099	1.00	30.52
2857	CG	LEU	B	784	40.599	43.447	43.895	1.00	35.83
2858	CD1	LEU	B	784	40.345	42.533	45.087	1.00	36.58
2859	CD2	LEU	B	784	39.523	44.498	43.810	1.00	36.04
2860	N	ASN	B	785	44.237	46.761	43.912	1.00	25.22
2861	CA	ASN	B	785	45.625	47.017	44.306	1.00	30.59
2862	C	ASN	B	785	45.715	46.566	45.763	1.00	29.47
2863	O	ASN	B	785	44.688	46.271	46.387	1.00	30.15
2864	CB	ASN	B	785	46.018	48.501	44.155	1.00	25.33
2865	CG	ASN	B	785	45.043	49.451	44.824	1.00	29.56
2866	OD1	ASN	B	785	44.530	49.182	45.907	1.00	35.66
2867	ND2	ASN	B	785	44.815	50.590	44.193	1.00	30.74
2868	N	GLU	B	786	46.918	46.509	46.321	1.00	30.15
2869	CA	GLU	B	786	47.051	46.007	47.684	1.00	29.94
2870	C	GLU	B	786	46.168	46.734	48.691	1.00	30.50
2871	O	GLU	B	786	45.591	46.100	49.572	1.00	30.06
2872	CB	GLU	B	786	48.527	46.011	48.132	1.00	34.17
2873	CG	GLU	B	786	48.744	45.444	49.540	1.00	33.86
2874	CD	GLU	B	786	50.188	45.061	49.836	1.00	41.39
2875	OE1	GLU	B	786	51.113	45.780	49.403	1.00	34.83
2876	OE2	GLU	B	786	50.399	44.042	50.530	1.00	40.62
2877	N	GLN	B	787	46.051	48.051	48.569	1.00	32.42
2878	CA	GLN	B	787	45.205	48.804	49.499	1.00	35.44
2879	C	GLN	B	787	43.748	48.337	49.417	1.00	34.61
2880	O	GLN	B	787	43.051	48.231	50.430	1.00	31.06
2881	CB	GLN	B	787	45.267	50.303	49.195	1.00	33.37
2882	CG	GLN	B	787	44.361	51.147	50.096	1.00	42.09
2883	CD	GLN	B	787	44.724	51.049	51.571	1.00	48.86
2884	OE1	GLN	B	787	43.991	51.537	52.435	1.00	55.24
2885	NE2	GLN	B	787	45.861	50.430	51.864	1.00	49.14
2886	N	ARG	B	788	43.283	48.065	48.206	1.00	31.38
2887	CA	ARG	B	788	41.909	47.625	48.043	1.00	34.58
2888	C	ARG	B	788	41.784	46.219	48.645	1.00	32.19

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2889	O	ARG	B	788	40.755	45.872	49.240	1.00	35.75
	2890	CB	ARG	B	788	41.524	47.641	46.570	1.00	26.45
	2891	CG	ARG	B	788	40.034	47.506	46.356	1.00	37.78
10	2892	CD	ARG	B	788	39.652	47.601	44.891	1.00	43.22
	2893	NE	ARG	B	788	38.202	47.526	44.738	1.00	40.59
	2894	CZ	ARG	B	788	37.560	47.561	43.577	1.00	46.17
15	2895	NH1	ARG	B	788	38.236	47.671	42.438	1.00	45.32
	2896	NH2	ARG	B	788	36.233	47.491	43.563	1.00	47.99
	2897	N	MET	B	789	42.841	45.420	48.505	1.00	34.27
20	2898	CA	MET	B	789	42.865	44.072	49.068	1.00	30.67
	2899	C	MET	B	789	42.757	44.175	50.583	1.00	37.95
	2900	O	MET	B	789	41.995	43.451	51.220	1.00	33.50
25	2901	CB	MET	B	789	44.184	43.352	48.774	1.00	31.27
	2902	CG	MET	B	789	44.522	43.165	47.317	1.00	30.70
	2903	SD	MET	B	789	46.045	42.194	47.093	1.00	32.85
30	2904	CE	MET	B	789	46.482	42.698	45.419	1.00	29.49
	2905	N	LYS	B	790	43.545	45.076	51.157	1.00	35.89
	2906	CA	LYS	B	790	43.574	45.250	52.605	1.00	40.34
35	2907	C	LYS	B	790	42.210	45.644	53.187	1.00	41.10
	2908	O	LYS	B	790	41.873	45.255	54.309	1.00	41.11
	2909	CB	LYS	B	790	44.642	46.290	52.948	1.00	38.07
40	2910	CG	LYS	B	790	45.016	46.402	54.411	1.00	46.09
	2911	CD	LYS	B	790	46.202	47.357	54.572	1.00	50.19
	2912	CE	LYS	B	790	47.419	46.859	53.795	1.00	53.06
45	2913	NZ	LYS	B	790	48.594	47.781	53.878	1.00	61.09
	2914	N	GLU	B	791	41.425	46.397	52.418	1.00	42.50
	2915	CA	GLU	B	791	40.097	46.848	52.848	1.00	45.42
50	2916	C	GLU	B	791	38.974	45.916	52.374	1.00	45.11
	2917	O	GLU	B	791	37.797	46.271	52.456	1.00	46.15
	2918	CB	GLU	B	791	39.812	48.248	52.281	1.00	45.54
55	2919	CG	GLU	B	791	40.788	49.343	52.711	1.00	51.32
	2920	CD	GLU	B	791	40.477	50.691	52.075	1.00	53.09
	2921	OE1	GLU	B	791	39.310	51.129	52.147	1.00	59.60
55	2922	OE2	GLU	B	791	41.400	51.326	51.520	1.00	53.82
	2923	N	SER	B	792	39.324	44.726	51.897	1.00	43.25
	2924	CA	SER	B	792	38.325	43.803	51.344	1.00	45.29
	2925	C	SER	B	792	37.463	42.934	52.267	1.00	45.71

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2926	O	SER	B	792	36.291	42.696	51.966	48.47
	2927	CB	SER	B	792	39.004	42.886	50.321	41.92
	2928	OG	SER	B	792	39.956	42.038	50.946	37.83
10	2929	N	SER	B	793	38.060	42.456	53.359	47.99
	2930	CA	SER	B	793	37.444	41.566	54.352	44.28
	2931	C	SER	B	793	38.058	40.181	54.126	45.52
	2932	O	SER	B	793	37.939	39.278	54.967	38.10
15	2933	CB	SER	B	793	35.909	41.484	54.229	52.05
	2934	OG	SER	B	793	35.503	40.710	53.110	51.73
	2935	N	PHE	B	794	38.709	40.011	52.975	36.75
20	2936	CA	PHE	B	794	39.383	38.752	52.674	34.46
	2937	C	PHE	B	794	40.815	38.977	52.193	35.15
	2938	O	PHE	B	794	41.285	38.344	51.245	29.12
	2939	CB	PHE	B	794	38.597	37.897	51.659	34.09
25	2940	CG	PHE	B	794	38.136	38.638	50.435	31.82
	2941	CD1	PHE	B	794	37.005	39.454	50.480	34.38
	2942	CD2	PHE	B	794	38.807	38.487	49.227	33.70
30	2943	CE1	PHE	B	794	36.546	40.108	49.336	32.42
	2944	CE2	PHE	B	794	38.358	39.141	48.070	35.10
	2945	CZ	PHE	B	794	37.227	39.951	48.127	33.58
	2946	N	TYR	B	795	41.503	39.884	52.884	35.15
35	2947	CA	TYR	B	795	42.895	40.227	52.584	36.03
	2948	C	TYR	B	795	43.759	38.970	52.496	29.03
	2949	O	TYR	B	795	44.546	38.810	51.558	30.92
40	2950	CB	TYR	B	795	43.446	41.148	53.682	33.87
	2951	CG	TYR	B	795	44.860	41.666	53.462	42.87
	2952	CD1	TYR	B	795	45.405	41.771	52.179	45.74
	2953	CD2	TYR	B	795	45.636	42.091	54.540	43.44
45	2954	CE1	TYR	B	795	46.689	42.287	51.979	46.16
	2955	CE2	TYR	B	795	46.914	42.605	54.353	49.66
	2956	CZ	TYR	B	795	47.436	42.700	53.071	51.20
50	2957	OH	TYR	B	795	48.707	43.199	52.884	51.61
	2958	N	SER	B	796	43.609	38.065	53.458	29.71
	2959	CA	SER	B	796	44.432	36.855	53.463	33.41
	2960	C	SER	B	796	44.262	36.003	52.210	34.99
55	2961	O	SER	B	796	45.228	35.433	51.697	30.81
	2962	CB	SER	B	796	44.128	36.004	54.696	32.48

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	2963	OG	SER	B	796	42.764	35.641	54.718	1.00	46.57
	2964	N	LEU	B	797	43.031	35.919	51.720	1.00	31.82
	2965	CA	LEU	B	797	42.768	35.135	50.521	1.00	34.40
10	2966	C	LEU	B	797	43.399	35.854	49.342	1.00	27.87
	2967	O	LEU	B	797	43.963	35.224	48.451	1.00	31.27
	2968	CB	LEU	B	797	41.261	35.000	50.291	1.00	31.93
15	2969	CG	LEU	B	797	40.858	33.875	49.334	1.00	37.66
	2970	CD1	LEU	B	797	41.251	32.542	49.949	1.00	36.98
	2971	CD2	LEU	B	797	39.362	33.900	49.106	1.00	38.90
20	2972	N	CYS	B	798	43.292	37.179	49.337	1.00	31.24
	2973	CA	CYS	B	798	43.885	37.980	48.271	1.00	30.70
	2974	C	CYS	B	798	45.377	37.723	48.202	1.00	29.69
25	2975	O	CYS	B	798	45.912	37.508	47.120	1.00	28.98
	2976	CB	CYS	B	798	43.620	39.468	48.492	1.00	30.81
	2977	SG	CYS	B	798	41.896	39.959	48.184	1.00	34.74
30	2978	N	LEU	B	799	46.057	37.738	49.344	1.00	30.05
	2979	CA	LEU	B	799	47.499	37.467	49.350	1.00	31.95
	2980	C	LEU	B	799	47.804	36.066	48.826	1.00	34.28
35	2981	O	LEU	B	799	48.771	35.862	48.090	1.00	31.99
	2982	CB	LEU	B	799	48.078	37.608	50.756	1.00	37.86
	2983	CG	LEU	B	799	47.990	39.005	51.366	1.00	40.98
40	2984	CD1	LEU	B	799	48.504	38.957	52.806	1.00	39.48
	2985	CD2	LEU	B	799	48.799	39.996	50.528	1.00	38.01
	2986	N	THR	B	800	46.991	35.089	49.214	1.00	32.31
45	2987	CA	THR	B	800	47.200	33.722	48.749	1.00	31.22
	2988	C	THR	B	800	47.153	33.664	47.230	1.00	28.73
	2989	O	THR	B	800	47.970	32.990	46.587	1.00	31.25
50	2990	CB	THR	B	800	46.125	32.774	49.338	1.00	32.96
	2991	OG1	THR	B	800	46.392	32.603	50.729	1.00	37.48
	2992	CG2	THR	B	800	46.121	31.414	48.638	1.00	31.79
55	2993	N	MET	B	801	46.196	34.372	46.648	1.00	27.39
	2994	CA	MET	B	801	46.078	34.376	45.206	1.00	25.92
	2995	C	MET	B	801	47.190	35.190	44.553	1.00	28.37
55	2996	O	MET	B	801	47.715	34.804	43.516	1.00	26.82
	2997	CB	MET	B	801	44.725	34.938	44.794	1.00	30.43
	2998	CG	MET	B	801	43.567	33.998	45.053	1.00	25.00
	2999	SD	MET	B	801	42.026	34.755	44.543	1.00	39.28

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	3000	CE	MET	B	801	41.910	36.095	45.721	1.00	31.74
	3001	N	TRP	B	802	47.555	36.301	45.180	1.00	27.61
	3002	CA	TRP	B	802	48.574	37.204	44.656	1.00	29.01
10	3003	C	TRP	B	802	49.942	36.527	44.503	1.00	31.69
	3004	O	TRP	B	802	50.812	37.016	43.773	1.00	31.46
	3005	CB	TRP	B	802	48.640	38.429	45.574	1.00	28.86
15	3006	CG	TRP	B	802	49.311	39.628	45.007	1.00	29.63
	3007	CD1	TRP	B	802	49.528	39.914	43.686	1.00	30.48
	3008	CD2	TRP	B	802	49.716	40.781	45.738	1.00	27.02
20	3009	NE1	TRP	B	802	50.040	41.184	43.554	1.00	26.74
	3010	CE2	TRP	B	802	50.163	41.738	44.800	1.00	30.15
	3011	CE3	TRP	B	802	49.740	41.102	47.100	1.00	27.81
25	3012	CZ2	TRP	B	802	50.630	42.990	45.182	1.00	29.45
	3013	CZ3	TRP	B	802	50.207	42.356	47.479	1.00	31.99
	3014	CH2	TRP	B	802	50.643	43.282	46.521	1.00	30.34
30	3015	N	GLN	B	803	50.118	35.386	45.164	1.00	31.67
	3016	CA	GLN	B	803	51.371	34.641	45.081	1.00	33.58
	3017	C	GLN	B	803	51.638	34.097	43.676	1.00	37.24
35	3018	O	GLN	B	803	52.787	33.878	43.293	1.00	33.37
	3019	CB	GLN	B	803	51.365	33.465	46.061	1.00	35.29
	3020	CG	GLN	B	803	51.335	33.839	47.539	1.00	45.49
40	3021	CD	GLN	B	803	51.288	32.611	48.447	1.00	46.24
	3022	OE1	GLN	B	803	52.138	31.728	48.355	1.00	55.28
	3023	NE2	GLN	B	803	50.293	32.557	49.327	1.00	53.88
45	3024	N	ILE	B	804	50.587	33.867	42.900	1.00	27.44
	3025	CA	ILE	B	804	50.789	33.320	41.567	1.00	28.71
	3026	C	ILE	B	804	51.477	34.279	40.612	1.00	22.83
50	3027	O	ILE	B	804	52.439	33.906	39.951	1.00	28.57
	3028	CB	ILE	B	804	49.454	32.854	40.947	1.00	24.30
	3029	CG1	ILE	B	804	48.854	31.748	41.819	1.00	30.72
55	3030	CG2	ILE	B	804	49.692	32.334	39.531	1.00	32.39
	3031	CD1	ILE	B	804	47.479	31.293	41.391	1.00	28.78
	3032	N	PRO	B	805	50.969	35.514	40.493	1.00	26.89
	3033	CA	PRO	B	805	51.627	36.449	39.577	1.00	29.13
	3034	C	PRO	B	805	53.055	36.778	40.018	1.00	33.32
	3035	O	PRO	B	805	53.924	37.035	39.193	1.00	32.54
	3036	CB	PRO	B	805	50.684	37.654	39.588	1.00	31.35

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3037	CG	PRO	B	805	50.099	37.602	40.969	1.00	34.40
	3038	CD	PRO	B	805	49.762	36.125	41.070	1.00	27.20
	3039	N	GLN	B	806	53.302	36.745	41.319	1.00	32.34
10	3040	CA	GLN	B	806	54.637	37.050	41.809	1.00	36.70
	3041	C	GLN	B	806	55.569	35.922	41.367	1.00	39.30
	3042	O	GLN	B	806	56.774	36.124	41.175	1.00	37.37
15	3043	CB	GLN	B	806	54.623	37.180	43.338	1.00	37.55
	3044	CG	GLN	B	806	53.654	38.230	43.899	1.00	40.88
	3045	CD	GLN	B	806	53.948	39.660	43.444	1.00	48.76
20	3046	OE1	GLN	B	806	53.279	40.605	43.870	1.00	53.24
	3047	NE2	GLN	B	806	54.943	39.824	42.583	1.00	42.24
	3048	N	GLU	B	807	54.999	34.735	41.178	1.00	32.14
25	3049	CA	GLU	B	807	55.791	33.593	40.764	1.00	35.89
	3050	C	GLU	B	807	56.033	33.651	39.260	1.00	32.99
	3051	O	GLU	B	807	57.071	33.198	38.781	1.00	34.50
30	3052	CB	GLU	B	807	55.086	32.293	41.150	1.00	40.93
	3053	CG	GLU	B	807	55.989	31.087	41.147	1.00	44.91
	3054	CD	GLU	B	807	57.191	31.280	42.051	1.00	55.41
35	3055	OE1	GLU	B	807	57.002	31.627	43.239	1.00	58.81
	3056	OE2	GLU	B	807	58.327	31.082	41.575	1.00	62.55
	3057	N	PHE	B	808	55.076	34.203	38.517	1.00	32.23
40	3058	CA	PHE	B	808	55.230	34.345	37.068	1.00	29.01
	3059	C	PHE	B	808	56.333	35.382	36.832	1.00	31.50
	3060	O	PHE	B	808	57.128	35.246	35.914	1.00	32.70
45	3061	CB	PHE	B	808	53.933	34.841	36.420	1.00	29.87
	3062	CG	PHE	B	808	52.870	33.786	36.279	1.00	29.41
	3063	CD1	PHE	B	808	53.146	32.454	36.546	1.00	34.35
50	3064	CD2	PHE	B	808	51.594	34.135	35.857	1.00	30.60
	3065	CE1	PHE	B	808	52.156	31.472	36.395	1.00	40.92
	3066	CE2	PHE	B	808	50.599	33.174	35.701	1.00	27.80
55	3067	CZ	PHE	B	808	50.877	31.842	35.970	1.00	29.99
	3068	N	VAL	B	809	56.366	36.420	37.665	1.00	36.56
	3069	CA	VAL	B	809	57.391	37.459	37.543	1.00	36.76
55	3070	C	VAL	B	809	58.743	36.800	37.770	1.00	40.16
	3071	O	VAL	B	809	59.673	36.949	36.965	1.00	40.88
	3072	CB	VAL	B	809	57.190	38.585	38.592	1.00	38.00
	3073	CG1	VAL	B	809	58.409	39.520	38.615	1.00	39.88

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	3074	CG2	VAL	B	809	55.944	39.390	38.251	1.00	34.92
	3075	N	LYS	B	810	58.831	36.044	38.857	1.00	35.81
	3076	CA	LYS	B	810	60.059	35.365	39.223	1.00	39.66
10	3077	C	LYS	B	810	60.589	34.395	38.176	1.00	40.69
	3078	O	LYS	B	810	61.783	34.396	37.887	1.00	39.53
	3079	CB	LYS	B	810	59.875	34.633	40.549	1.00	44.11
15	3080	CG	LYS	B	810	61.103	33.854	40.995	1.00	50.84
	3081	CD	LYS	B	810	60.917	33.255	42.385	1.00	58.43
	3082	CE	LYS	B	810	60.773	34.341	43.448	1.00	56.52
20	3083	NZ	LYS	B	810	60.552	33.768	44.812	1.00	61.40
	3084	N	LEU	B	811 1	59.707	33.570	37.612	1.00	37.80
	3085	CA	LEU	B	811	60.107	32.596	36.601	1.00	38.18
25	3086	C	LEU	B	811	60.127	33.145	35.183	1.00	37.73
	3087	O	LEU	B	811	60.578	32.469	34.258	1.00	37.38
	3088	CB	LEU	B	811 1	59.168	31.392	36.631	1.00	41.71
30	3089	CG	LEU	B	811	59.188	30.533	37.889	1.00	43.91
	3090	CD1	LEU	B	811	58.114	29.464	37.790	1.00	47.64
	3091	CD2	LEU	B	811	60.562	29.901	38.041	1.00	47.76
35	3092	N	GLN	B	812	59.627	34.362	35.012	1.00	36.65
	3093	CA	GLN	B	812	59.564	34.979	33.693	1.00	38.46
	3094	C	GLN	B	812	58.839	34.031	32.724	1.00	35.35
40	3095	O	GLN	B	812	59.291	33.786	31.607	1.00	33.66
	3096	CB	GLN	B	812	60.983	35.281	33.206	1.00	46.92
	3097	CG	GLN	B	812	61.763	36.139	34.196	1.00	52.42
45	3098	CD	GLN	B	812	63.241	36.277	33.852	1.00	62.75
	3099	OE1	GLN	B	812	63.995	36.928	34.579	1.00	62.90
	3100	NE2	GLN	B	812	63.661	35.662	32.746	1.00	62.19
50	3101	N	VAL	B	813	57.706	33.496	33.166	1.00	33.05
	3102	CA	VAL	B	813	56.928	32.577	32.334	1.00	30.09
	3103	C	VAL	B	813	56.559	33.219	31.005	1.00	26.61
55	3104	O	VAL	B	813	56.136	34.374	30.948	1.00	27.45
	3105	CB	VAL	B	813	55.645	32.126	33.063	1.00	32.65
	3106	CG1	VAL	B	813	54.816	31.198	32.158	1.00	32.05
55	3107	CG2	VAL	B	813	56.024	31.405	34.332	1.00	31.32
	3108	N	SER	B	814	56.745	32.469	29.924	1.00	28.74
	3109	CA	SER	B	814	56.415	32.982	28.599	1.00	26.63
	3110	C	SER	B	814	54.972	32.609	28.307	1.00	25.32

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3111	O	SER	B	814	54.413	31.720	28.945	1.00	26.17
	3112	CB	SER	B	814	57.291	32.338	27.537	1.00	20.76
	3113	OG	SER	B	814	57.087	30.930	27.530	1.00	32.55
10	3114	N	GLN	B	815	54.387	33.290	27.332	1.00	29.06
	3115	CA	GLN	B	815	53.014	33.031	26.931	1.00	30.84
	3116	C	GLN	B	815	52.858	31.597	26.438	1.00	30.78
15	3117	O	GLN	B	815	51.800	30.983	26.614	1.00	29.76
	3118	CB	GLN	B	815	52.613	34.010	25.825	1.00	33.76
	3119	CG	GLN	B	815	51.168	33.883	25.367	1.00	48.56
20	3120	CD	GLN	B	815	50.791	34.935	24.337	1.00	53.59
	3121	OE1	GLN	B	815	50.880	36.139	24.595	1.00	61.73
	3122	NE2	GLN	B	815	50.370	34.487	23.167	1.00	53.05
25	3123	N	GLU	B	816	53.914	31.062	25.821	1.00	28.64
	3124	CA	GLU	B	816	53.886	29.709	25.294	1.00	26.48
	3125	C	GLU	B	816	53.873	28.657	26.400	1.00	28.37
30	3126	O	GLU	B	816	53.181	27.647	26.297	1.00	26.00
	3127	CB	GLU	B	816	55.090	29.464	24.370	1.00	28.52
	3128	CG	GLU	B	816	55.187	30.379	23.135	1.00	30.85
35	3129	CD	GLU	B	816	55.387	31.853	23.474	1.00	40.74
	3130	OE1	GLU	B	816	56.191	32.155	24.380	1.00	35.62
	3131	OE2	GLU	B	816	54.756	32.718	22.821	1.00	48.10
40	3132	N	GLU	B	817	54.646	28.875	27.458	1.00	28.18
	3133	CA	GLU	B	817	54.679	27.908	28.561	1.00	22.67
	3134	C	GLU	B	817	53.334	27.952	29.308	1.00	26.65
45	3135	O	GLU	B	817	52.798	26.912	29.718	1.00	27.82
	3136	CB	GLU	B	817	55.827	28.253	29.508	1.00	31.49
	3137	CG	GLU	B	817	57.197	28.222	28.815	1.00	30.28
50	3138	CD	GLU	B	817	58.301	28.832	29.664	1.00	41.20
	3139	OE1	GLU	B	817	58.072	29.918	30.242	1.00	33.70
	3140	OE2	GLU	B	817	59.403	28.243	29.730	1.00	35.22
55	3141	N	PHE	B	818	52.812	29.162	29.470	1.00	22.36
	3142	CA	PHE	B	818	51.535	29.410	30.140	1.00	25.25
	3143	C	PHE	B	818	50.392	28.641	29.484	1.00	24.77
55	3144	O	PHE	B	818	49.610	27.981	30.167	1.00	24.06
	3145	CB	PHE	B	818	51.196	30.903	30.087	1.00	22.70
	3146	CG	PHE	B	818	49.781	31.227	30.526	1.00	24.41
	3147	CD1	PHE	B	818	49.388	31.042	31.845	1.00	24.27

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	3148	CD2	PHE	B	818	48.846	31.703	29.612	1.00	29.17
	3149	CE1	PHE	B	818	48.077	31.321	32.256	1.00	27.63
	3150	CE2	PHE	B	818	47.530	31.985	30.006	1.00	31.24
10	3151	CZ	PHE	B	818	47.147	31.794	31.329	1.00	27.17
	3152	N	LEU	B	819	50.299	28.728	28.158	1.00	26.67
	3153	CA	LEU	B	819	49.220	28.053	27.434	1.00	21.35
15	3154	C	LEU	B	819	49.221	26.540	27.594	1.00	30.98
	3155	O	LEU	B	819	48.158	25.926	27.736	1.00	23.62
	3156	CB	LEU	B	819	49.259	28.437	25.953	1.00	29.60
20	3157	CG	LEU	B	819	48.936	29.911 1	25.692	1.00	22.84
	3158	CD1	LEU	B	819	49.334	30.306	24.285	1.00	30.19
	3159	CD2	LEU	B	819	47.459	30.156	25.931	1.00	31.22
25	3160	N	CYS	B	820	50.399	25.931	27.572	1.00	22.63
	3161	CA	CYS	B	820	50.491	24.489	27.755	1.00	28.50
	3162	C	CYS	B	820	50.171	24.127	29.200	1.00	26.00
30	3163	O	CYS	B	820	49.458	23.144	29.465	1.00	24.25
	3164	CB	CYS	B	820	51.896	23.993	27.406	1.00	27.91
	3165	SG	CYS	B	820	52.317	24.170	25.661	1.00	32.47
35	3166	N	MET	B	821	50.707	24.913	30.135	1.00	22.36
	3167	CA	MET	B	821	50.483	24.654	31.556	1.00	21.33
	3168	C	MET	B	821	49.015	24.778	31.898	1.00	26.26
40	3169	O	MET	B	821	48.503	24.021	32.715	1.00	25.87
	3170	CB	MET	B	821	51.278	25.626	32.433	1.00	26.99
	3171	CG	MET	B	821	52.782	25.421	32.382	1.00	28.60
45	3172	SD	MET	B	821	53.621	26.820	33.184	1.00	34.96
	3173	CE	MET	B	821	53.294	26.479	34.906	1.00	34.63
	3174	N	LYS	B	822	48.334	25.721	31.267	1.00	22.01
50	3175	CA	LYS	B	822	46.923	25.884	31.562	1.00	24.77
	3176	C	LYS	B	822	46.135	24.647	31.126	1.00	24.24
	3177	O	LYS	B	822	45.188	24.221	31.804	1.00	20.06
55	3178	CB	LYS	B	822	46.396	27.164	30.901	1.00	22.46
	3179	CG	LYS	B	822	44.991	27.512	31.372	1.00	25.45
	3180	CD	LYS	B	822	44.675	28.996	31.201	1.00	34.91
55	3181	CE	LYS	B	822	44.712	29.433	29.753	1.00	38.39
	3182	NZ	LYS	B	822	43.654	28.750	28.981	1.00	37.51
	3183	N	VAL	B	823	46.532	24.043	30.007	1.00	22.51
	3184	CA	VAL	B	823	45.852	22.831	29.546	1.00	19.35

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3185	C	VAL	B	823	46.140	21.700	30.511 1	1.00	20.40
	3186	O	VAL	B	823	45.266	20.879	30.822	1.00	18.38
	3187	CB	VAL	B	823	46.316	22.387	28.147	1.00	17.40
10	3188	CG1	VAL	B	823	45.663	21.037	27.785	1.00	23.17
	3189	CG2	VAL	B	823	45.910	23.426	27.129	1.00	25.04
	3190	N	LEU	B	824	47.372	21.657	31.012	1.00	20.55
15	3191	CA	LEU	B	824	47.705	20.611	31.951	1.00	21.76
	3192	C	LEU	B	824	46.874	20.734	33.230	1.00	19.28
	3193	O	LEU	B	824	46.540	19.721	33.837	1.00	22.64
20	3194	CB	LEU	B	824	49.210	20.610	32.245	1.00	22.31
	3195	CG	LEU	B	824	50.058	20.144	31.047	1.00	22.09
	3196	CD1	LEU	B	824	51.548	20.248	31.388	1.00	32.05
25	3197	CD2	LEU	B	824	49.668	18.707	30.684	1.00	23.33
	3198	N	LEU	B	825	46.511	21.956	33.619	1.00	21.54
	3199	CA	LEU	B	825	45.684	22.134	34.814	1.00	21.16
30	3200	C	LEU	B	825	44.304	21.500	34.594	1.00	22.24
	3201	O	LEU	B	825	43.757	20.858	35.483	1.00	20.01
	3202	CB	LEU	B	825	45.547	23.614	35.164	1.00	19.34
35	3203	CG	LEU	B	825	46.814	24.203	35.786	1.00	22.57
	3204	CD1	LEU	B	825	46.629	25.698	36.063	1.00	22.91
	3205	CD2	LEU	B	825	47.101	23.450	37.096	1.00	22.94
40	3206	N	LEU	B	826	43.750	21.674	33.403	1.00	21.69
	3207	CA	LEU	B	826	42.465	21.067	33.072	1.00	21.95
	3208	C	LEU	B	826	42.544	19.533	33.192	1.00	24.10
45	3209	O	LEU	B	826	41.552	18.865	33.499	1.00	23.49
	3210	CB	LEU	B	826	42.072	21.462	31.637	1.00	20.89
	3211 1	CG	LEU	B	826	40.832	20.808	31.017	1.00	23.40
50	3212	CD1	LEU	B	826	39.543	21.272	31.757	1.00	21.60
	3213	CD2	LEU	B	826	40.759	21.198	29.532	1.00	21.37
	3214	N	LEU	B	827	43.727	18.973	32.953	1.00	21.74
55	3215	CA	LEU	B	827	43.902	17.531	32.999	1.00	26.22
	3216	C	LEU	B	827	44.732	17.087	34.208	1.00	26.34
	3217	O	LEU	B	827	45.374	16.041	34.157	1.00	27.08
55	3218	CB	LEU	B	827	44.620	17.081	31.715	1.00	23.15
	3219	CG	LEU	B	827	44.092	17.626	30.388	1.00	25.05
	3220	CD1	LEU	B	827	45.027	17.213	29.229	1.00	23.87
	3221	CD2	LEU	B	827	42.672	17.097	30.180	1.00	24.70

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3222	N	ASN	B	828	44.702	17.855	35.295	1.00	26.63
	3223	CA	ASN	B	828	45.531	17.537	36.466	1.00	23.58
	3224	C	ASN	B	828	44.887	16.756	37.625	1.00	26.70
10	3225	O	ASN	B	828	45.534	16.519	38.639	1.00	25.23
	3226	CB	ASN	B	828	46.130	18.838	37.025	1.00	28.11
	3227	CG	ASN	B	828	47.592	18.685	37.418	1.00	37.40
15	3228	OD1	ASN	B	828	48.159	19.529	38.113	1.00	38.18
	3229	ND2	ASN	B	828	48.213	17.617	36.947	1.00	33.20
	3230	N	THR	B	829	43.621	16.377	37.499	1.00	23.98
20	3231	CA	THR	B	829	42.938	15.622	38.552	1.00	23.70
	3232	C	THR	B	829	41.947	14.683	37.866	1.00	25.10
	3233	O	THR	B	829	41.250	15.100	36.952	1.00	25.89
25	3234	CB	THR	B	829	42.133	16.555	39.496	1.00	24.60
	3235	OG1	THR	B	829	42.984	17.586	40.006	1.00	28.70
	3236	CG2	THR	B	829	41.557	15.760	40.661	1.00	28.67
30	3237	N	ILE	B	830	41.887	13.427	38.295	1.00	22.29
	3238	CA	ILE	B	830	40.969	12.442	37.715	1.00	24.53
	3239	C	ILE	B	830	40.210	11.721	38.848	1.00	24.95
35	3240	O	ILE	B	830	40.627	11.783	40.005	1.00	20.63
	3241	CB	ILE	B	830	41.795	11.428	36.877	1.00	28.68
	3242	CG1	ILE	B	830	42.571	12.177	35.799	1.00	30.48
40	3243	CG2	ILE	B	830	40.913	10.426	36.194	1.00	36.11
	3244	CD1	ILE	B	830	41.689	12.930	34.851	1.00	43.97
	3245	N	PRO	B	831	39.067	11.070	38.544	1.00	23.25
45	3246	CA	PRO	B	831	38.351	10.377	39.616	1.00	24.91
	3247	C	PRO	B	831	39.232	9.258	40.168	1.00	31.60
	3248	O	PRO	B	831	40.238	8.897	39.558	1.00	30.37
50	3249	CB	PRO	B	831	37.122	9.822	38.900	1.00	29.20
	3250	CG	PRO	B	831	36.909	10.831	37.777	1.00	27.01
	3251	CD	PRO	B	831	38.324	10.924	37.277	1.00	22.94
55	3252	N	LEU	B	832	38.863	8.724	41.325	1.00	29.91
	3253	CA	LEU	B	832	39.632	7.630	41.911	1.00	35.35
	3254	C	LEU	B	832	39.541	6.396	41.017	1.00	34.24
55	3255	O	LEU	B	832	40.499	5.638	40.898	1.00	42.02
	3256	CB	LEU	B	832	39.103	7.304	43.312	1.00	31.75
	3257	CG	LEU	B	832	39.307	8.462	44.291	1.00	37.36
	3258	CD1	LEU	B	832	38.703	8.121	45.640	1.00	38.79

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3259	CD2	LEU	B	832	40.793	8.762	44.419	1.00	38.51
	3260	N	GLU	B	833	38.394	6.223	40.369	1.00	37.07
	3261	CA	GLU	B	833	38.157	5.079	39.495	1.00	40.48
10	3262	C	GLU	B	833	38.648	5.346	38.078	1.00	36.29
	3263	O	GLU	B	833	38.431	4.532	37.177	1.00	39.85
	3264	CB	GLU	B	833	36.656	4.756	39.435	1.00	43.67
15	3265	CG	GLU	B	833	35.832	5.259	40.620	1.00	59.82
	3266	CD	GLU	B	833	35.634	6.772	40.595	1.00	59.36
	3267	OE1	GLU	B	833	34.979	7.261	39.652	1.00	65.43
20	3268	OE2	GLU	B	833	36.135	7.471	41.502	1.00	61.15
	3269	N	GLY	B	834	39.307	6.481	37.880	1.00	33.66
	3270	CA	GLY	B	834	39.783	6.828	36.558	1.00	32.35
25	3271	C	GLY	B	834	38.640	7.338	35.694	1.00	29.12
	3272	O	GLY	B	834	37.489	7.379	36.128	1.00	28.18
	3273	N	LEU	B	835	38.954	7.719	34.468	1.00	28.73
30	3274	CA	LEU	B	835	37.947	8.228	33.532	1.00	31.82
	3275	C	LEU	B	835	37.397	7.131	32.613	1.00	30.35
	3276	O	LEU	B	835	37.987	6.058	32.503	1.00	33.32
35	3277	CB	LEU	B	835	38.579	9.312	32.671	1.00	25.42
	3278	CG	LEU	B	835	39.101	10.535	33.411	1.00	28.35
	3279	CD1	LEU	B	835	40.019	11.335	32.491	1.00	26.14
40	3280	CD2	LEU	B	835	37.935	11.374	33.882	1.00	25.47
	3281	N	ARG	B	836	36.283	7.405	31.938	1.00	32.23
	3282	CA	ARG	B	836	35.721	6.422	31.012	1.00	33.49
45	3283	C	ARG	B	836	36.602	6.367	29.764	1.00	32.90
	3284	O	ARG	B	836	36.700	5.328	29.102	1.00	35.77
	3285	CB	ARG	B	836	34.290	6.787	30.629	1.00	32.58
50	3286	CG	ARG	B	836	33.302	6.699	31.780	1.00	45.22
	3287	CD	ARG	B	836	31.880	6.883	31.280	1.00	50.46
	3288	NE	ARG	B	836	31.554	5.891	30.254	1.00	63.72
55	3289	CZ	ARG	B	836	30.366	5.771	29.671	1.00	61.91
	3290	NH1	ARG	B	836	29.372	6.586	30.004	1.00	64.45
	3291	NH2	ARG	B	836	30.173	4.837	28.748	1.00	68.06
	3292	N	SER	B	837	37.237	7.490	29.445	1.00	27.88
	3293	CA	SER	B	837	38.130	7.577	28.297	1.00	30.32
	3294	C	SER	B	837	39.564	7.712	28.814	1.00	29.09
	3295	O	SER	B	837	40.341	8.538	28.353	1.00	25.31

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	3296	CB	SER	B	837	37.758	8.785	27.431	1.00	33.53
	3297	OG	SER	B	837	36.408	8.698	26.991	1.00	32.13
	3298	N	GLN	B	838	39.912	6.867	29.772	1.00	32.66
10	3299	CA	GLN	B	838	41.242	6.907	30.355	1.00	30.97
	3300	C	GLN	B	838	42.377	6.811	29.330	1.00	32.88
	3301	O	GLN	B	838	43.378	7.515	29.448	1.00	29.00
15	3302	CB	GLN	B	838	41.392	5.798	31.402	1.00	37.64
	3303	CG	GLN	B	838	42.645	5.953	32.253	1.00	34.77
	3304	CD	GLN	B	838	42.619	7.213	33.117	1.00	42.70
20	3305	OE1	GLN	B	838	43.665	7.713	33.533	1.00	43.05
	3306	NE2	GLN	B	838	41.424	7.718	33.404	1.00	40.24
	3307	N	THR	B	839	42.236	5.957	28.320	1.00	32.29
25	3308	CA	THR	B	839	43.291	5.829	27.321	1.00	32.08
	3309	C	THR	B	839	43.495	7.122	26.538	1.00	30.37
	3310	O	THR	B	839	44.623	7.583	26.369	1.00	27.02
30	3311 1	CB	THR	B	839	42.994	4.685	26.316	1.00	36.84
	3312	OG1	THR	B	839	42.914	3.442	27.021	1.00	33.01
	3313	CG2	THR	B	839	44.106	4.593	25.253	1.00	34.47
35	3314	N	GLN	B	840	42.403	7.709	26.057	1.00	27.73
	3315	CA	GLN	B	840	42.501	8.945	25.292	1.00	28.34
	3316	C	GLN	B	840	43.027	10.070	26.168	1.00	28.06
40	3317	O	GLN	B	840	43.735	10.963	25.700	1.00	26.67
	3318	CB	GLN	B	840	41.142	9.339	24.711	1.00	32.45
	3319	CG	GLN	B	840	40.481	8.269	23.836	1.00	46.64
45	3320	CD	GLN	B	840	39.661	7.236	24.617	1.00	53.33
	3321	OE1	GLN	B	840	40.172	6.514	25.478	1.00	44.62
	3322	NE2	GLN	B	840	38.370	7.169	24.306	1.00	55.68
50	3323	N	PHE	B	841	42.666	10.021	27.444	1.00	24.94
	3324	CA	PHE	B	841	43.108	11.018	28.397	1.00	27.01
	3325	C	PHE	B	841	44.619	10.962	28.540	1.00	23.28
55	3326	O	PHE	B	841	45.293	11.981	28.443	1.00	22.03
	3327	CB	PHE	B	841	42.480	10.769	29.767	1.00	25.37
	3328	CG	PHE	B	841	43.038	11.651	30.844	1.00	22.03
55	3329	CD1	PHE	B	841	42.632	12.965	30.962	1.00	26.46
	3330	CD2	PHE	B	841	44.005	11.166	31.719	1.00	26.10
	3331	CE1	PHE	B	841	43.174	13.799	31.937	1.00	25.57
	3332	CE2	PHE	B	841	44.561	11.995	32.703	1.00	25.36

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3333	CZ	PHE	B	841	44.141	13.313	32.808	1.00	25.63
	3334	N	GLU	B	842	45.152	9.770	28.781	1.00	27.54
	3335	CA	GLU	B	842	46.607	9.639	28.939	1.00	29.02
10	3336	C	GLU	B	842	47.347	10.143	27.717	1.00	25.06
	3337	O	GLU	B	842	48.357	10.826	27.837	1.00	27.55
	3338	CB	GLU	B	842	47.010	8.183	29.199	1.00	36.85
15	3339	CG	GLU	B	842	46.593	7.628	30.568	1.00	46.79
	3340	CD	GLU	B	842	47.223	8.376	31.741	1.00	50.21
	3341	OE1	GLU	B	842	47.948	9.364	31.510	1.00	51.33
20	3342	OE2	GLU	B	842	46.987	7.974	32.901	1.00	54.97
	3343	N	GLU	B	843	46.849	9.795	26.535	1.00	27.99
	3344	CA	GLU	B	843	47.484	10.235	25.302	1.00	29.91
25	3345	C	GLU	B	843	47.455	11.750	25.197	1.00	24.87
	3346	O	GLU	B	843	48.445	12.375	24.829	1.00	25.77
	3347	CB	GLU	B	843	46.788	9.619	24.084	1.00	33.71
30	3348	CG	GLU	B	843	46.809	8.087	24.081	1.00	43.17
	3349	CD	GLU	B	843	46.362	7.487	22.761	1.00	47.10
	3350	OE1	GLU	B	843	46.082	8.258	21.822	1.00	53.30
35	3351	OE2	GLU	B	843	46.304	6.241	22.656	1.00	50.03
	3352	N	MET	B	844	46.319	12.345	25.542	1.00	25.91
	3353	CA	MET	B	844	46.168	13.787	25.468	1.00	23.10
40	3354	C	MET	B	844	47.064	14.475	26.490	1.00	22.35
	3355	O	MET	B	844	47.746	15.454	26.184	1.00	23.84
	3356	CB	MET	B	844	44.711	14.182	25.722	1.00	24.04
45	3357	CG	MET	B	844	44.442	15.681	25.592	1.00	27.46
	3358	SD	MET	B	844	42.709	16.055	26.067	1.00	29.20
	3359	CE	MET	B	844	42.699	17.809	25.977	1.00	22.37
50	3360	N	ARG	B	845	47.046	13.975	27.716	1.00	25.23
	3361	CA	ARG	B	845	47.887	14.574	28.740	1.00	29.00
	3362	C	ARG	B	845	49.353	14.423	28.345	1.00	27.50
55	3363	O	ARG	B	845	50.121	15.372	28.446	1.00	25.08
	3364	CB	ARG	B	845	47.613	13.934	30.101	1.00	27.08
	3365	CG	ARG	B	845	48.367	14.594	31.240	1.00	37.67
	3366	CD	ARG	B	845	47.781	14.196	32.586	1.00	36.90
	3367	NE	ARG	B	845	48.525	14.771	33.705	1.00	51.09
	3368	CZ	ARG	B	845	49.746	14.390	34.063	1.00	42.11
	3369	NH1	ARG	B	845	50.363	13.422	33.400	1.00	50.54

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3407	CB	ARG	B	850	55.255	15.957	24.226	1.00	26.91
	3408	CG	ARG	B	850	55.521	14.511	24.663	1.00	27.09
	3409	CD	ARG	B	850	55.646	13.575	23.458	1.00	29.81
10	3410	NE	ARG	B	850	54.413	13.394	22.686	1.00	31.76
	3411	CZ	ARG	B	850	53.402	12.598	23.037	1.00	31.98
	3412	NH1	ARG	B	850	53.448	11.880	24.160	1.00	35.55
15	3413	NH2	ARG	B	850	52.340	12.504	22.254	1.00	34.47
	3414	N	GLU	B	851	54.242	19.018	24.620	1.00	27.13
	3415	CA	GLU	B	851	54.133	20.358	24.029	1.00	22.10
20	3416	C	GLU	B	851	54.765	21.378	24.987	1.00	27.46
	3417	O	GLU	B	851	55.394	22.347	24.551	1.00	29.77
	3418	CB	GLU	B	851	52.664	20.719	23.761	1.00	30.54
25	3419	CG	GLU	B	851	52.505	21.829	22.716	1.00	32.90
	3420	CD	GLU	B	851	53.026	21.401	21.338	1.00	42.32
	3421	OE1	GLU	B	851	53.314	20.191	21.155	1.00	33.77
30	3422	OE2	GLU	B	851	53.140	22.266	20.439	1.00	34.60
	3423	N	LEU	B	852	54.587	21.168	26.293	1.00	23.76
	3424	CA	LEU	B	852	55.204	22.064	27.265	1.00	26.78
35	3425	C	LEU	B	852	56.726	22.019	27.067	1.00	22.14
	3426	O	LEU	B	852	57.399	23.046	27.101	1.00	26.98
	3427	CB	LEU	B	852	54.879	21.625	28.687	1.00	22.84
40	3428	CG	LEU	B	852	55.560	22.451	29.782	1.00	26.06
	3429	CD1	LEU	B	852	55.271	23.923	29.577	1.00	23.63
	3430	CD2	LEU	B	852	55.080	21.993	31.145	1.00	26.99
45	3431	N	ILE	B	853	57.251	20.810	26.876	1.00	28.61
	3432	CA	ILE	B	853	58.689	20.628	26.690	1.00	24.00
	3433	C	ILE	B	853	59.166	21.389	25.458	1.00	27.59
50	3434	O	ILE	B	853	60.267	21.929	25.453	1.00	29.87
	3435	CB	ILE	B	853	59.031	19.136	26.574	1.00	26.82
	3436	CG1	ILE	B	853	58.737	18.458	27.919	1.00	25.90
55	3437	CG2	ILE	B	853	60.478	18.972	26.104	1.00	24.70
	3438	CD1	ILE	B	853	58.685	16.935	27.876	1.00	23.86
	3439	N	LYS	B	854	58.343	21.442	24.411	1.00	24.04
55	3440	CA	LYS	B	854	58.725	22.192	23.215	1.00	28.78
	3441	C	LYS	B	854	58.668	23.690	23.497	1.00	28.51
	3442	O	LYS	B	854	59.508	24.457	23.020	1.00	29.04
	3443	CB	LYS	B	854	57.788	21.893	22.039	1.00	29.18

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3444	CG	LYS	B	854	57.765	20.460	21.555	1.00	33.70
	3445	CD	LYS	B	854	56.758	20.366	20.418	1.00	35.70
	3446	CE	LYS	B	854	56.587	18.960	19.913	1.00	48.12
10	3447	NZ	LYS	B	854	55.515	18.932	18.876	1.00	43.84
	3448	N	ALA	B	855	57.661	24.112	24.256	1.00	28.37
	3449	CA	ALA	B	855	57.504	25.535	24.592	1.00	25.35
15	3450	C	ALA	B	855	58.719	26.035	25.379	1.00	26.32
	3451	O	ALA	B	855	59.203	27.156	25.185	1.00	25.77
	3452	CB	ALA	B	855	56.218	25.745	25.417	1.00	29.46
20	3453	N	ILE	B	856	59.194	25.204	26.292	1.00	27.24
	3454	CA	ILE	B	856	60.361	25.562	27.073	1.00	27.67
	3455	C	ILE	B	856	61.543	25.659	26.100	1.00	34.93
25	3456	O	ILE	B	856	62.414	26.522	26.230	1.00	30.85
	3457	CB	ILE	B	856	60.672	24.481	28.116	1.00	30.91
	3458	CG1	ILE	B	856	59.582	24.474	29.197	1.00	30.70
30	3459	CG2	ILE	B	856	62.060	24.718	28.725	1.00	30.32
	3460	CD1	ILE	B	856	59.729	23.310	30.188	1.00	28.42
	3461	N	GLY	B	857	61.540	24.771	25.113	1.00	32.68
35	3462	CA	GLY	B	857	62.618	24.739	24.141	1.00	37.55
	3463	C	GLY	B	857	62.769	26.010	23.330	1.00	39.78
	3464	O	GLY	B	857	63.836	26.269	22.777	1.00	38.63
40	3465	N	LEU	B	858	61.712	26.809	23.257	1.00	42.53
	3466	CA	LEU	B	858	61.747	28.048	22.486	1.00	44.50
	3467	C	LEU	B	858	62.711	29.110	23.012	1.00	49.32
45	3468	O	LEU	B	858	63.281	29.877	22.236	1.00	47.44
	3469	CB	LEU	B	858	60.344	28.649	22.405	1.00	45.48
	3470	CG	LEU	B	858	59.304	27.814	21.663	1.00	42.37
50	3471	CD1	LEU	B	858	57.941	28.491	21.752	1.00	47.24
	3472	CD2	LEU	B	858	59.733	27.651	20.217	1.00	47.70
	3473	N	ARG	B	859	62.887	29.171	24.323	1.00	51.14
55	3474	CA	ARG	B	859	63.774	30.170	24.899	1.00	60.57
	3475	C	ARG	B	859	64.948	29.538	25.620	1.00	63.51
	3476	O	ARG	B	859	66.088	29.648	25.172	1.00	66.86
	3477	CB	ARG	B	859	62.994	31.080	25.852	1.00	60.03
	3478	CG	ARG	B	859	61.946	31.931	25.147	1.00	66.28
	3479	CD	ARG	B	859	61.112	32.750	26.120	1.00	65.17
	3480	NE	ARG	B	859	60.150	33.601	25.422	1.00	72.22

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3481	CZ	ARG	B	859	59.228	33.155	24.573	1.00	75.01
	3482	NH1	ARG	B	859	59.134	31.857	24.305	1.00	74.54
	3483	NH2	ARG	B	859	58.394	34.006	23.990	1.00	77.06
10	3484	N	GLN	B	860	64.670	28.876	26.736	1.00	67.91
	3485	CA	GLN	B	860	65.730	28.235	27.492	1.00	67.91
	3486	C	GLN	B	860	66.514	27.268	26.623	1.00	70.16
15	3487	O	GLN	B	860	66.108	26.124	26.403	1.00	66.29
	3488	CB	GLN	B	860	65.167	27.527	28.731	1.00	68.82
	3489	CG	GLN	B	860	64.975	28.461	29.925	1.00	70.16
20	3490	CD	GLN	B	860	63.978	29.584	29.675	1.00	73.18
	3491	OE1	GLN	B	860	63.922	30.553	30.434	1.00	75.31
	3492	NE2	GLN	B	860	63.172	29.449	28.629	1.00	74.53
25	3493	N	LYS	B	861	67.636	27.766	26.110	1.00	70.28
	3494	CA	LYS	B	861	68.527	26.982	25.274	1.00	70.98
	3495	C	LYS	B	861	69.480	26.247	26.205	1.00	69.66
30	3496	O	LYS	B	861	70.017	26.833	27.149	1.00	69.56
	3497	CB	LYS	B	861	69.334	27.889	24.342	1.00	73.98
	3498	CG	LYS	B	861	68.512	28.696	23.352	1.00	76.75
35	3499	CD	LYS	B	861	67.728	27.806	22.403	1.00	79.85
	3500	CE	LYS	B	861	67.077	28.623	21.296	1.00	82.15
	3501	NZ	LYS	B	861	66.190	29.694	21.820	1.00	83.45
40	3502	N	GLY	B	862	69.687	24.964	25.942	1.00	65.51
	3503	CA	GLY	B	862	70.581	24.187	26.777	1.00	62.36
	3504	C	GLY	B	862	69.870	23.045	27.473	1.00	58.94
45	3505	O	GLY	B	862	68.786	23.219	28.027	1.00	55.70
	3506	N	VAL	B	863	70.496	21.874	27.450	1.00	55.20
	3507	CA	VAL	B	863	69.934	20.680	28.063	1.00	54.32
50	3508	C	VAL	B	863	69.691	20.830	29.567	1.00	52.94
	3509	O	VAL	B	863	68.643	20.436	30.070	1.00	51.71
	3510	CB	VAL	B	863	70.850	19.461	27.812	1.00	53.87
55	3511	CG1	VAL	B	863	72.228	19.710	28.406	1.00	54.75
	3512	CG2	VAL	B	863	70.228	18.212	28.405	1.00	55.92
	3513	N	VAL	B	864	70.651	21.404	30.282	1.00	51.96
55	3514	CA	VAL	B	864	70.513	21.578	31.725	1.00	50.09
	3515	C	VAL	B	864	69.445	22.622	32.065	1.00	49.79
	3516	O	VAL	B	864	68.577	22.383	32.903	1.00	46.15
	3517	CB	VAL	B	864	71.864	22.001	32.372	1.00	50.90

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3518	CG1	VAL	B	864	71.740	21.991	33.889	1.00	49.47
	3519	CG2	VAL	B	864	72.973	21.056	31.936	1.00	46.98
	3520	N	SER	B	865	69.504	23.772	31.403	1.00	43.87
10	3521	CA	SER	B	865	68.539	24.830	31.653	1.00	46.16
	3522	C	SER	B	865	67.124	24.366	31.314	1.00	43.21
	3523	O	SER	B	865	66.178	24.660	32.045	1.00	41.52
15	3524	CB	SER	B	865	68.893	26.066	30.828	1.00	46.68
	3525	OG	SER	B	865	68.014	27.136	31.116	1.00	59.14
	3526	N	SER	B	866	66.988	23.628	30.215	1.00	40.92
20	3527	CA	SER	B	866	65.682	23.139	29.776	1.00	35.24
	3528	C	SER	B	866	65.071	22.097	30.695	1.00	40.63
	3529	O	SER	B	866	63.874	22.154	30.980	1.00	32.01
25	3530	CB	SER	B	866	65.772	22.565	28.362	1.00	37.02
	3531	OG	SER	B	866	66.142	23.573	27.443	1.00	45.95
	3532	N	SER	B	867	65.877	21.134	31.146	1.00	37.03
30	3533	CA	SER	B	867	65.372	20.099	32.040	1.00	36.93
	3534	C	SER	B	867	65.077	20.710	33.407	1.00	40.17
	3535	O	SER	B	867	64.149	20.282	34.099	1.00	35.95
35	3536	CB	SER	B	867	66.382	18.952	32.187	1.00	40.92
	3537	OG	SER	B	867	67.556	19.387	32.850	1.00	48.34
	3538	N	GLN	B	868	65.872	21.697	33.810	1.00	37.09
40	3539	CA	GLN	B	868	65.623	22.354	35.093	1.00	41.94
	3540	C	GLN	B	868	64.340	23.189	35.025	1.00	34.5 ₅
	3541	O	GLN	B	868	63.579	23.242	35.990	1.00	35.43
45	3542	CB	GLN	B	868	66.790	23.267	35.490	1.00	43.10
	3543	CG	GLN	B	868	68.042	22.519	35.954	1.00	54.16
	3544	CD	GLN	B	868	69.125	23.450	36.495	1.00	59.01
50	3545	OE1	GLN	B	868	70.155	22.994	36.992	1.00	60.70
	3546	NE2	GLN	B	868	68.893	24.759	36.399	1.00	59.00
	3547	N	ARG	B	869	64.112	23.847	33.893	1.00	34.25
55	3548	CA	ARG	B	869	62.918	24.666	33.746	1.00	32.37
	3549	C	ARG	B	869	61.673	23.778	33.716	1.00	33.17
	3550	O	ARG	B	869	60.633	24.147	34.262	1.00	32.22
55	3551	CB	ARG	B	869	63.001	25.541	32.500	1.00	34.11
	3552	CG	ARG	B	869	61.908	26.619	32.493	1.00	39.35
	3553	CD	ARG	B	869	62.127	27.633	31.406	1.00	42.79
	3554	NE	ARG	B	869	61.101	28.672	31.368	1.00	40.15

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3555	CZ	ARG	B	869	60.828	29.522	32.350	1.00	39.72
	3556	NH1	ARG	B	869	61.502	29.478	33.492	1.00	43.65
	3557	NH2	ARG	B	869	59.867	30.425	32.185	1.00	36.33
10	3558	N	PHE	B	870	61.781	22.601	33.101	1.00	30.79
	3559	CA	PHE	B	870	60.670	21.651	33.078	1.00	30.15
	3560	C	PHE	B	870	60.299	21.259	34.516	1.00	35.55
15	3561	O	PHE	B	870	59.117	21.156	34.857	1.00	30.41
	3562	CB	PHE	B	870	61.042	20.373	32.330	1.00	34.17
	3563	CG	PHE	B	870	59.923	19.373	32.263	1.00	31.63
20	3564	CD1	PHE	B	870	58.818	19.607	31.449	1.00	34.59
	3565	CD2	PHE	B	870	59.949	18.225	33.041	1.00	36.46
	3566	CE1	PHE	B	870	57.758	18.715	31.412	1.00	34.87
25	3567	CE2	PHE	B	870	58.887	17.322	33.012	1.00	42.81
	3568	CZ	PHE	B	870	57.789	17.569	32.195	1.00	35.48
	3569	N	TYR	B	871	61.305	21.021	35.358	1.00	28.70
30	3570	CA	TYR	B	871	61.029	20.653	36.746	1.00	32.21
	3571	C	TYR	B	871	60.381	21.809	37.513	1.00	31.93
	3572	O	TYR	B	871	59.464	21.590	38.313	1.00	32.87
35	3573	CB	TYR	B	871	62.314	20.183	37.459	1.00	33.96
	3574	CG	TYR	B	871	62.117	19.878	38.930	1.00	37.15
	3575	CD1	TYR	B	871	62.099	20.902	39.883	1.00	44.42
40	3576	CD2	TYR	B	871	61.895	18.571	39.368	1.00	45.79
	3577	CE1	TYR	B	871	61.863	20.632	41.233	1.00	42.43
	3578	CE2	TYR	B	871	61.657	18.289	40.722	1.00	47.61
45	3579	CZ	TYR	B	871	61.641	19.326	41.646	1.00	50.61
	3580	OH	TYR	B	871	61.393	19.061	42.978	1.00	55.59
	3581	N	GLN	B	872	60.853	23.032	37.268	1.00	29.65
50	3582	CA	GLN	B	872	60.298	24.216	37.935	1.00	32.37
	3583	C	GLN	B	872	58.832	24.460	37.566	1.00	31.80
	3584	O	GLN	B	872	57.986	24.675	38.444	1.00	28.10
55	3585	CB	GLN	B	872	61.075	25.476	37.568	1.00	29.72
	3586	CG	GLN	B	872	62.498	25.554	38.096	1.00	42.15
	3587	CD	GLN	B	872	63.207	26.805	37.605	1.00	43.54
55	3588	OE1	GLN	B	872	63.427	26.978	36.405	1.00	48.46
	3589	NE2	GLN	B	872	63.554	27.690	38.529	1.00	54.30
	3590	N	LEU	B	873	58.541	24.449	36.267	1.00	30.13
	3591	CA	LEU	B	873	57.176	24.686	35.806	1.00	30.27

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3592	C	LEU	B	873	56.205	23.598	36.234	1.00	35.12
3593	O	LEU	B	873	55.051	23.889	36.590	1.00	32.42
3594	CB	LEU	B	873	57.146	24.876	34.284	1.00	31.46
3595	CG	LEU	B	873	57.871	26.154	33.836	1.00	25.50
3596	CD1	LEU	B	873	57.739	26.342	32.322	1.00	26.12
3597	CD2	LEU	B	873	57.293	27.359	34.569	1.00	30.31
3598	N	THR	B	874	56.650	22.348	36.208	1.00	32.47
3599	CA	THR	B	874	55.777	21.274	36.631	1.00	31.43
3600	C	THR	B	874	55.664	21.315	38.158	1.00	33.30
3601	O	THR	B	874	54.610	21.009	38.713	1.00	32.00
3602	CB	THR	B	874	56.292	19.883	36.157	1.00	33.76
3603	OG1	THR	B	874	57.628	19.683	36.610	1.00	36.17
3604	CG2	THR	B	874	56.261	19.788	34.628	1.00	31.16
3605	N	LYS	B	875	56.736	21.710	38.842	1.00	31.72
3606	CA	LYS	B	875	56.677	21.780	40.303	1.00	35.19
3607	C	LYS	B	875	55.701	22.895	40.688	1.00	33.68
3608	O	LYS	B	875	54.983	22.794	41.686	1.00	33.61
3609	CB	LYS	B	875	58.062	22.067	40.907	1.00	37.62
3610	CG	LYS	B	875	58.091	21.945	42.429	1.00	40.41
3611	CD	LYS	B	875	57.761	20.509	42.843	1.00	43.28
3612	CE	LYS	B	875	57.618	20.357	44.354	1.00	41.31
3613	NZ	LYS	B	875	57.273	18.939	44.712	1.00	45.62
3614	N	LEU	B	876	55.682	23.958	39.890	1.00	30.46
3615	CA	LEU	B	876	54.782	25.081	40.129	1.00	34.18
3616	C	LEU	B	876	53.345	24.568	40.037	1.00	33.33
3617	O	LEU	B	876	52.510	24.892	40.881	1.00	32.77
3618	CB	LEU	B	876	55.026	26.179	39.093	1.00	35.40
3619	CG	LEU	B	876	54.302	27.520	39.218	1.00	35.72
3620	CD1	LEU	B	876	54.848	28.485	38.179	1.00	42.08
3621	CD2	LEU	B	876	52.806	27.336	39.039	1.00	42.68
3622	N	LEU	B	877	53.060	23.754	39.022	1.00	29.58
3623	CA	LEU	B	877	51.721	23.208	38.869	1.00	30.87
3624	C	LEU	B	877	51.345	22.311	40.053	1.00	34.72
3625	O	LEU	B	877	50.220	22.392	40.555	1.00	31.85
3626	CB	LEU	B	877	51.601	22.439	37.544	1.00	32.60
3627	CG	LEU	B	877	51.708	23.298	36.274	1.00	33.97
3628	CD1	LEU	B	877	51.665	22.424	35.020	1.00	29.88

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3629	CD2	LEU	B	877	50.565	24.314	36.268	1.00	34.90
	3630	N	ASP	B	878	52.274	21.463	40.505	1.00	30.56
	3631	CA	ASP	B	878	51.995	20.576	41.647	1.00	32.09
10	3632	C	ASP	B	878	51.659	21.415	42.872	1.00	26.56
	3633	O	ASP	B	878	50.754	21.079	43.642	1.00	29.15
	3634	CB	ASP	B	878	53.205	19.709	42.001	1.00	31.44
15	3635	CG	ASP	B	878	53.686	18.868	40.846	1.00	45.52
	3636	OD1	ASP	B	878	52.913	18.024	40.344	1.00	38.49
	3637	OD2	ASP	B	878	54.851	19.050	40.441	1.00	51.89
20	3638	N	ASN	B	879	52.411	22.491	43.061	1.00	26.43
	3639	CA	ASN	B	879	52.187	23.393	44.185	1.00	33.73
	3640	C	ASN	B	879	50.798	24.042	44.128	1.00	32.92
25	3641	O	ASN	B	879	50.233	24.391	45.163	1.00	33.36
	3642	CB	ASN	B	879	53.255	24.490	44.222	1.00	31.44
	3643	CG	ASN	B	879	54.604	23.989	44.705	1.00	41.99
30	3644	OD1	ASN	B	879	55.580	24.742	44.727	1.00	46.26
	3645	ND2	ASN	B	879	54.666	22.719	45.102	1.00	38.65
	3646	N	LEU	B	880	50.247	24.216	42.931	1.00	32.60
35	3647	CA	LEU	B	880	48.919	24.821	42.818	1.00	33.43
	3648	C	LEU	B	880	47.832	24.063	43.566	1.00	33.86
	3649	O	LEU	B	880	46.878	24.669	44.045	1.00	32.44
40	3650	CB	LEU	B	880	48.499	24.979	41.354	1.00	37.74
	3651	CG	LEU	B	880	48.820	26.311	40.686	1.00	43.19
	3652	CD1	LEU	B	880	48.433	26.273	39.208	1.00	42.98
45	3653	CD2	LEU	B	880	48.053	27.410	41.416	1.00	43.09
	3654	N	HIS	B	881	47.960	22.745	43.659	1.00	34.37
	3655	CA	HIS	B	881	46.971	21.944	44.377	1.00	36.86
50	3656	C	HIS	B	881	46.746	22.467	45.791	1.00	38.92
	3657	O	HIS	B	881	45.613	22.620	46.232	1.00	38.03
	3658	CB	HIS	B	881	47.424	20.486	44.438	1.00	38.32
55	3659	CG	HIS	B	881	47.321	19.770	43.129	1.00	46.94
	3660	ND1	HIS	B	881	48.098	18.675	42.814	1.00	54.16
	3661	CD2	HIS	B	881	46.513	19.975	42.062	1.00	49.76
55	3662	CE1	HIS	B	881	47.775	18.237	41.611	1.00	49.51
	3663	NE2	HIS	B	881	46.814	19.008	41.132	1.00	56.41
	3664	N	ASP	B	882	47.839	22.741	46.491	1.00	36.82
	3665	CA	ASP	B	882	47.799	23.236	47.861	1.00	39.00

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3666	C	ASP	B	882	47.144	24.616	47.950	1.00	37.23
3667	O	ASP	B	882	46.325	24.876	48.833	1.00	38.12
3668	CB	ASP	B	882	49.229	23.324	48.397	1.00	48.17
3669	CG	ASP	B	882	50.038	22.075	48.099	1.00	57.26
3670	OD1	ASP	B	882	50.294	21.799	46.900	1.00	57.71
3671	OD2	ASP	B	882	50.409	21.362	49.058	1.00	65.58
3672	N	LEU	B	883	47.531	25.492	47.028	1.00	32.08
3673	CA	LEU	B	883	47.025	26.855	46.939	1.00	29.89
3674	C	LEU	B	883	45.527	26.833	46.637	1.00	31.31
3675	O	LEU	B	883	44.729	27.516	47.280	1.00	27.71
3676	CB	LEU	B	883	47.757	27.580	45.812	1.00	36.27
3677	CG	LEU	B	883	47.649	29.088	45.604	1.00	34.71
3678	CD1	LEU	B	883	46.197	29.517	45.367	1.00	37.86
3679	CD2	LEU	B	883	48.249	29.773	46.812	1.00	51.86
3680	N	VAL	B	884	45.154	26.047	45.639	1.00	26.92
3681	CA	VAL	B	884	43.757	25.940	45.248	1.00	24.81
3682	C	VAL	B	884	42.896	25.301	46.345	1.00	26.03
3683	O	VAL	B	884	41.712	25.600	46.473	1.00	22.11
3684	CB	VAL	B	884	43.640	25.139	43.938	1.00	29.47
3685	CG1	VAL	B	884	42.196	24.853	43.614	1.00	30.72
3686	CG2	VAL	B	884	44.278	25.944	42.805	1.00	30.08
3687	N	LYS	B	885	43.484	24.418	47.142	1.00	23.85
3688	CA	LYS	B	885	42.716	23.800	48.215	1.00	24.88
3689	C	LYS	B	885	42.189	24.905	49.145	1.00	25.51
3690	O	LYS	B	885	41.038	24.844	49.607	1.00	22.01
3691	CB	LYS	B	885	43.593	22.819	48.985	1.00	29.10
3692	CG	LYS	B	885	42.865	22.086	50.096	1.00	37.31
3693	CD	LYS	B	885	43.761	21.053	50.762	1.00	31.31
3694	CE	LYS	B	885	43.049	20.417	51.951	1.00	38.95
3695	NZ	LYS	B	885	43.916	19.437	52.668	1.00	41.49
3696	N	GLN	B	886	43.015	25.921	49.403	1.00	23.54
3697	CA	GLN	B	886	42.602	27.039	50.275	1.00	26.86
3698	C	GLN	B	886	41.428	27.822	49.684	1.00	29.25
3699	O	GLN	B	886	40.528	28.228	50.418	1.00	21.92
3700	CB	GLN	B	886	43.764	28.010	50.531	1.00	32.12
3701	CG	GLN	B	886	44.939	27.408	51.301	1.00	37.80
3702	CD	GLN	B	886	46.118	28.374	51.422	1.00	45.69

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3703	OE1	GLN	B	886	46.041	29.400	52.103	1.00	44.67
	3704	NE2	GLN	B	886	47.212	28.051	50.743	1.00	49.75
	3705	N	LEU	B	887	41.465	28.045	48.367	1.00	24.24
10	3706	CA	LEU	B	887	40.402	28.749	47.648	1.00	19.73
	3707	C	LEU	B	887	39.127	27.894	47.648	1.00	17.60
	3708	O	LEU	B	887	38.017	28.410	47.775	1.00	21.95
15	3709	CB	LEU	B	887	40.836	29.028	46.203	1.00	24.60
	3710	CG	LEU	B	887	42.047	29.951	46.027	1.00	25.31
	3711 1	CD1	LEU	B	887	42.369	30.108	44.543	1.00	26.29
20	3712	CD2	LEU	B	887	41.757	31.290	46.641	1.00	29.73
	3713	N	HIS	B	888	39.292	26.580	47.502	1.00	18.82
	3714	CA	HIS	B	888	38.165	25.649	47.513	1.00	18.69
25	3715	C	HIS	B	888	37.422	25.669	48.845	1.00	22.15
	3716	O	HIS	B	888	36.194	25.684	48.874	1.00	19.70
	3717	CB	HIS	B	888	38.654	24.228	47.247	1.00	20.05
30	3718	CG	HIS	B	888	38.877	23.923	45.796	1.00	22.81
	3719	ND1	HIS	B	888	39.526	22.784	45.370	1.00	26.59
	3720	CD2	HIS	B	888	38.459	24.559	44.674	1.00	23.24
35	3721	CE1	HIS	B	888	39.495	22.726	44.050	1.00	27.50
	3722	NE2	HIS	B	888	38.854	23.791	43.603	1.00	29.04
	3723	N	LEU	B	889	38.165	25.642	49.949	1.00	19.08
40	3724	CA	LEU	B	889	37.536	25.652	51.274	1.00	24.07
	3725	C	LEU	B	889	36.812	26.977	51.535	1.00	23.35
	3726	O	LEU	B	889	35.689	26.981	52.023	1.00	21.52
45	3727	CB	LEU	B	889	38.592	25.387	52.372	1.00	23.61
	3728	CG	LEU	B	889	38.105	25.401	53.835	1.00	23.63
	3729	CD1	LEU	B	889	36.945	24.430	54.022	1.00	25.11
50	3730	CD2	LEU	B	889	39.256	25.027	54.760	1.00	29.21
	3731	N	TYR	B	890	37.445	28.098	51.193	1.00	21.91
	3732	CA	TYR	B	890	36.828	29.408	51.404	1.00	23.79
55	3733	C	TYR	B	890	35.557	29.514	50.569	1.00	24.14
	3734	O	TYR	B	890	34.534	30.029	51.035	1.00	23.58
	3735	CB	TYR	B	890	37.813	30.531	51.026	1.00	25.81
55	3736	CG	TYR	B	890	37.301	31.930	51.332	1.00	26.23
	3737	CD1	TYR	B	890	36.308	32.528	50.547	1.00	23.51
	3738	CD2	TYR	B	890	37.781	32.636	52.432	1.00	29.47
	3739	CE1	TYR	B	890	35.813	33.793	50.861	1.00	26.90

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3740	CE2	TYR	B	890	37.284	33.906	52.749	1.00	29.33
3741	CZ	TYR	B	890	36.303	34.471	51.957	1.00	27.90
3742	OH	TYR	B	890	35.814	35.716	52.265	1.00	28.09
3743	N	CYS	B	891	35.628	29.017	49.336	1.00	22.38
3744	CA	CYS	B	891	34.491	29.045	48.438	1.00	22.23
3745	C	CYS	B	891	33.338	28.199	48.976	1.00	19.96
3746	O	CYS	B	891	32.212	28.669	49.064	1.00	19.08
3747	CB	CYS	B	891	34.923	28.550	47.055	1.00	26.16
3748	SG	CYS	B	891	33.587	28.353	45.863	1.00	25.55
3749	N	LEU	B	892	33.618	26.958	49.366	1.00	20.12
3750	CA	LEU	B	892	32.574	26.101	49.889	1.00	19.88
3751	C	LEU	B	892	31.936	26.685	51.159	1.00	20.91
3752	O	LEU	B	892	30.718	26.605	51.329	1.00	20.98
3753	CB	LEU	B	892	33.126	24.689	50.166	1.00	22.12
3754	CG	LEU	B	892	32.067	23.682	50.640	1.00	28.56
3755	CD1	LEU	B	892	30.955	23.585	49.580	1.00	23.62
3756	CD2	LEU	B	892	32.719	22.316	50.887	1.00	24.56
3757	N	ASN	B	893	32.744	27.262	52.052	1.00	19.36
3758	CA	ASN	B	893	32.199	27.855	53.275	1.00	21.31
3759	C	ASN	B	893	31.329	29.044	52.897	1.00	23.26
3760	O	ASN	B	893	30.288	29.269	53.501	1.00	22.28
3761	CB	ASN	B	893	33.308	28.363	54.200	1.00	22.90
3762	CG	ASN	B	893	33.988	27.262	54.986	1.00	27.81
3763	OD1	ASN	B	893	35.187	27.349	55.280	1.00	32.06
3764	ND2	ASN	B	893	33.230	26.245	55.370	1.00	26.08
3765	N	THR	B	894	31.762	29.818	51.901	1.00	20.27
3766	CA	THR	B	894	30.993	30.989	51.511	1.00	21.51
3767	C	THR	B	894	29.705	30.546	50.822	1.00	20.80
3768	O	THR	B	894	28.660	31.175	50.977	1.00	21.06
3769	CB	THR	B	894	31.818	31.925	50.593	1.00	20.63
3770	OG1	THR	B	894	32.987	32.359	51.301	1.00	25.68
3771	CG2	THR	B	894	31.015	33.171	50.218	1.00	23.83
3772	N	PHE	B	895	29.779	29.436	50.096	1.00	19.69
3773	CA	PHE	B	895	28.614	28.901	49.381	1.00	21.30
3774	C	PHE	B	895	27.538	28.436	50.380	1.00	23.16
3775	O	PHE	B	895	26.345	28.723	50.231	1.00	22.53
3776	CB	PHE	B	895	29.059	27.715	48.517	1.00	20.99

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3777	CG	PHE	B	895	27.968	27.127	47.686	1.00	24.35
	3778	CD1	PHE	B	895	27.422	27.842	46.613	1.00	25.21
	3779	CD2	PHE	B	895	27.467	25.864	47.979	1.00	27.79
10	3780	CE1	PHE	B	895	26.387	27.293	45.838	1.00	30.71
	3781	CE2	PHE	B	895	26.438	25.310	47.215	1.00	30.19
	3782	CZ	PHE	B	895	25.897	26.024	46.146	1.00	29.55
15	3783	N	ILE	B	896	27.972	27.703	51.390	1.00	20.73
	3784	CA	ILE	B	896	27.066	27.205	52.412	1.00	26.62
	3785	C	ILE	B	896	26.416	28.363	53.166	1.00	24.12
20	3786	O	ILE	B	896	25.234	28.309	53.499	1.00	25.34
	3787	CB	ILE	B	896	27.828	26.276	53.398	1.00	23.97
	3788	CG1	ILE	B	896	28.118	24.948	52.705	1.00	27.05
25	3789	CG2	ILE	B	896	27.028	26.063	54.683	1.00	34.01
	3790	CD1	ILE	B	896	28.991	24.019	53.510	1.00	34.75
	3791	N	GLN	B	897	27.173	29.427	53.403	1.00	19.74
30	3792	CA	GLN	B	897	26.645	30.573	54.145	1.00	23.53
	3793	C	GLN	B	897	26.204	31.724	53.237	1.00	25.84
	3794	O	GLN	B	897	26.002	32.848	53.713	1.00	26.80
35	3795	CB	GLN	B	897	27.722	31.081	55.111	1.00	26.51
	3796	CG	GLN	B	897	28.384	29.972	55.924	1.00	26.00
	3797	CD	GLN	B	897	29.571	30.449	56.734	1.00	34.46
40	3798	OE1	GLN	B	897	30.451	29.655	57.089	1.00	37.93
	3799	NE2	GLN	B	897	29.601	31.741	57.051	1.00	32.90
	3800	N	SER	B	898	26.014	31.448	51.950	1.00	24.26
45	3801	CA	SER	B	898	25.669	32.504	50.996	1.00	25.93
	3802	C	SER	B	898	24.543	33.449	51.402	1.00	29.21
	3803	O	SER	B	898	24.688	34.669	51.280	1.00	27.52
50	3804	CB	SER	B	898	25.364	31.917	49.613	1.00	23.86
	3805	OG	SER	B	898	24.312	30.991	49.687	1.00	31.50
	3806	N	ARG	B	899	23.433	32.904	51.896	1.00	24.74
55	3807	CA	ARG	B	899	22.307	33.752	52.292	1.00	32.34
	3808	C	ARG	B	899	22.650	34.720	53.425	1.00	29.89
	3809	O	ARG	B	899	22.342	35.910	53.355	1.00	33.92
60	3810	CB	ARG	B	899	21.103	32.902	52.733	1.00	31.79
	3811	CG	ARG	B	899	20.414	32.070	51.652	1.00	45.87
	3812	CD	ARG	B	899	19.077	31.532	52.204	1.00	50.81
65	3813	NE	ARG	B	899	18.248	30.819	51.231	1.00	61.64

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3814	CZ	ARG	B	899	17.821	31.324	50.075	1.00	63.01
3815	NH1	ARG	B	899	18.143	32.564	49.717	1.00	64.60
3816	NH2	ARG	B	899	17.052	30.589	49.281	1.00	64.49
3817	N	ALA	B	900	23.268	34.190	54.474	1.00	28.54
3818	CA	ALA	B	900	23.638	34.994	55.627	1.00	30.83
3819	C	ALA	B	900	24.669	36.051	55.269	1.00	35.27
3820	O	ALA	B	900	24.622	37.159	55.793	1.00	34.40
3821	CB	ALA	B	900	24.172	34.097	56.739	1.00	32.11
3822	N	LEU	B	901	25.580	35.720	54.354	1.00	30.18
3823	CA	LEU	B	901	26.628	36.645	53.939	1.00	32.20
3824	C	LEU	B	901	26.201	37.523	52.769	1.00	31.41
3825	O	LEU	B	901	26.950	38.401	52.343	1.00	34.81
3826	CB	LEU	B	901	27.873	35.861	53.525	1.00	32.10
3827	CG	LEU	B	901	28.546	34.937	54.535	1.00	35.51
3828	CD1	LEU	B	901	29.567	34.057	53.797	1.00	33.35
3829	CD2	LEU	B	901	29.207	35.746	55.635	1.00	35.37
3830	N	SER	B	902	25.008	37.271	52.236	1.00	29.08
3831	CA	SER	B	902	24.509	38.027	51.102	1.00	29.16
3832	C	SER	B	902	25.438	37.962	49.891	1.00	31.58
3833	O	SER	B	902	25.668	38.962	49.210	1.00	30.70
3834	CB	SER	B	902	24.278	39.488	51.505	1.00	35.73
3835	OG	SER	B	902	23.300	39.557	52.528	1.00	36.77
3836	N	VAL	B	903	25.991	36.779	49.641	1.00	28.81
3837	CA	VAL	B	903	26.857	36.572	48.486	1.00	28.11
3838	C	VAL	B	903	26.105	35.665	47.527	1.00	30.18
3839	O	VAL	B	903	25.799	34.521	47.851	1.00	37.08
3840	CB	VAL	B	903	28.183	35.891	48.870	1.00	28.45
3841	CG1	VAL	B	903	28.995	35.583	47.604	1.00	24.13
3842	CG2	VAL	B	903	28.998	36.809	49.759	1.00	23.64
3843	N	GLU	B	904	25.805	36.172	46.343	1.00	31.59
3844	CA	GLU	B	904	25.071	35.398	45.357	1.00	30.24
3845	C	GLU	B	904	25.993	34.542	44.497	1.00	33.23
3846	O	GLU	B	904	27.037	35.010	44.044	1.00	26.56
3847	CB	GLU	B	904	24.266	36.343	44.458	1.00	35.02
3848	CG	GLU	B	904	23.432	35.672	43.382	1.00	51.21
3849	CD	GLU	B	904	22.339	34.783	43.942	1.00	58.61
3850	OE1	GLU	B	904	22.664	33.733	44.538	1.00	68.45

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3851	OE2	GLU	B	904	21.149	35.143	43.794	1.00	71.56
	3852	N	PHE	B	905	25.614	33.280	44.303	1.00	25.33
	3853	CA	PHE	B	905	26.370	32.386	43.446	1.00	26.30
10	3854	C	PHE	B	905	25.461	32.046	42.280	1.00	25.19
	3855	O	PHE	B	905	24.367	31.507	42.482	1.00	25.92
	3856	CB	PHE	B	905	26.742	31.073	44.142	1.00	26.58
15	3857	CG	PHE	B	905	27.856	31.188	45.123	1.00	22.37
	3858	CD1	PHE	B	905	27.645	31.738	46.378	1.00	21.31
	3859	CD2	PHE	B	905	29.122	30.730	44.789	1.00	24.52
20	3860	CE1	PHE	B	905	28.668	31.834	47.296	1.00	20.76
	3861	CE2	PHE	B	905	30.175	30.818	45.703	1.00	23.76
	3862	CZ	PHE	B	905	29.946	31.370	46.958	1.00	25.94
25	3863	N	PRO	B	906	25.893	32.367	41.049	1.00	25.13
	3864	CA	PRO	B	906	25.175	32.120	39.800	1.00	28.59
	3865	C	PRO	B	906	24.942	30.642	39.577	1.00	25.62
30	3866	O	PRO	B	906	25.586	29.792	40.193	1.00	27.37
	3867	CB	PRO	B	906	26.109	32.722	38.751	1.00	28.96
	3868	CG	PRO	B	906	26.762	33.836	39.512	1.00	32.34
35	3869	CD	PRO	B	906	27.148	33.074	40.753	1.00	30.32
	3870	N	GLU	B	907	24.030	30.353	38.663	1.00	29.57
	3871	CA	GLU	B	907	23.615	28.999	38.312	1.00	30.56
40	3872	C	GLU	B	907	24.705	27.965	38.011	1.00	30.16
	3873	O	GLU	B	907	24.777	26.925	38.671	1.00	28.20
	3874	CB	GLU	B	907	22.673	29.097	37.111	1.00	39.44
45	3875	CG	GLU	B	907	21.926	27.827	36.761	1.00	50.34
	3876	CD	GLU	B	907	21.408	27.863	35.333	1.00	55.65
	3877	OE1	GLU	B	907	20.837	28.902	34.929	1.00	53.82
50	3878	OE2	GLU	B	907	21.573	26.850	34.620	1.00	56.79
	3879	N	MET	B	908	25.537	28.224	37.005	1.00	27.50
	3880	CA	MET	B	908	26.574	27.262	36.650	1.00	31.75
55	3881	C	MET	B	908	27.625	27.095	37.732	1.00	28.93
	3882	O	MET	B	908	28.143	26.002	37.931	1.00	27.45
	3883	CB	MET	B	908	27.259	27.633	35.326	1.00	36.79
55	3884	CG	MET	B	908	26.604	27.048	34.088	1.00	47.60
	3885	SD	MET	B	908	27.569	27.345	32.563	1.00	70.60
	3886	CE	MET	B	908	29.148	26.536	32.931	1.00	48.34
	3887	N	MET	B	909	27.933	28.175	38.437	1.00	26.74

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3888	CA	MET	B	909	28.929	28.095	39.483	1.00	29.95
3889	C	MET	B	909	28.379	27.233	40.620	1.00	27.02
3890	O	MET	B	909	29.084	26.393	41.186	1.00	25.18
3891	CB	MET	B	909	29.277	29.500	39.966	1.00	29.74
3892	CG	MET	B	909	30.506	29.555	40.836	1.00	39.86
3893	SD	MET	B	909	31.104	31.254	40.979	1.00	43.66
3894	CE	MET	B	909	32.567	30.954	41.943	1.00	40.49
3895	N	SER	B	910	27.109	27.429	40.954	1.00	27.09
3896	CA	SER	B	910	26.511	26.632	42.015	1.00	25.16
3897	C	SER	B	910	26.487	25.178	41.595	1.00	25.86
3898	O	SER	B	910	26.669	24.286	42.416	1.00	23.23
3899	CB	SER	B	910	25.091	27.106	42.305	1.00	24.90
3900	OG	SER	B	910	25.101	28.461	42.699	1.00	26.02
3901	N	GLU	B	911	26.255	24.935	40.308	1.00	25.46
3902	CA	GLU	B	911	26.215	23.567	39.809	1.00	29.55
3903	C	GLU	B	911	27.564	22.863	39.976	1.00	29.76
3904	O	GLU	B	911	27.620	21.769	40.536	1.00	28.96
3905	CB	GLU	B	911	25.808	23.531	38.330	1.00	34.77
3906	CG	GLU	B	911	25.935	22.134	37.708	1.00	51.59
3907	CD	GLU	B	911	25.725	22.110	36.199	1.00	56.41
3908	OE1	GLU	B	911	26.448	22.834	35.476	1.00	67.40
3909	OE2	GLU	B	911	24.845	21.355	35.734	1.00	66.05
3910	N	VAL	B	912	28.644	23.474	39.494	1.00	25.36
3911 1	CA	VAL	B	912	29.959	22.850	39.619	1.00	29.35
3912	C	VAL	B	912	30.381	22.701	41.075	1.00	26.61
3913	O	VAL	B	912	31.067	21.740	41.429	1.00	29.13
3914	CB	VAL	B	912	31.097	23.635	38.865	1.00	29.04
3915	CG1	VAL	B	912	30.780	23.735	37.383	1.00	29.38
3916	CG2	VAL	B	912	31.285	25.015	39.470	1.00	27.40
3917	N	ILE	B	913	29.972	23.642	41.919	1.00	26.12
3918	CA	ILE	B	913	30.325	23.589	43.328	1.00	26.31
3919	C	ILE	B	913	29.612	22.421	44.012	1.00	27.59
3920	O	ILE	B	913	30.220	21.644	44.760	1.00	24.84
3921	CB	ILE	B	913	29.979	24.931	44.024	1.00	28.04
3922	CG1	ILE	B	913	30.936	26.019	43.514	1.00	22.84
3923	CG2	ILE	B	913	30.048	24.773	45.559	1.00	25.12
3924	CD1	ILE	B	913	30.622	27.421	43.977	1.00	19.77

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3925	N	ALA	B	914	28.327	22.272	43.725	1.00	29.75
	3926	CA	ALA	B	914	27.547	21.194	44.323	1.00	26.87
	3927	C	ALA	B	914	27.931	19.836	43.770	1.00	29.99
10	3928	O	ALA	B	914	27.840	18.824	44.464	1.00	28.80
	3929	CB	ALA	B	914	26.047	21.440	44.098	1.00	28.77
	3930	N	ALA	B	915	28.372	19.794	42.521	1.00	27.03
15	3931	CA	ALA	B	915	28.718	18.514	41.917	1.00	27.59
	3932	C	ALA	B	915	30.015	17.884	42.383	1.00	28.38
	3933	O	ALA	B	915	30.111	16.664	42.427	1.00	34.38
20	3934	CB	ALA	B	915	28.733	18.633	40.389	1.00	24.76
	3935	N	GLN	B	916	31.007	18.689	42.735	1.00	25.09
	3936	CA	GLN	B	916	32.291	18.118	43.124	1.00	26.91
25	3937	C	GLN	B	916	33.073	18.705	44.293	1.00	25.33
	3938	O	GLN	B	916	33.931	18.022	44.863	1.00	29.86
	3939	CB	GLN	B	916	33.226	18.133	41.909	1.00	23.65
30	3940	CG	GLN	B	916	32.752	17.337	40.694	1.00	30.20
	3941	CD	GLN	B	916	32.436	15.889	41.034	1.00	30.77
	3942	OE1	GLN	B	916	33.180	15.235	41.756	1.00	36.33
35	3943	NE2	GLN	B	916	31.331	15.383	40.503	1.00	45.24
	3944	N	LEU	B	917	32.810	19.951	44.665	1.00	27.46
	3945	CA	LEU	B	917	33.629	20.558	45.700	1.00	23.85
40	3946	C	LEU	B	917	33.803	19.765	46.998	1.00	26.12
	3947	O	LEU	B	917	34.930	19.611	47.484	1.00	23.20
	3948	CB	LEU	B	917	33.148	21.987	45.970	1.00	32.48
45	3949	CG	LEU	B	917	34.234	22.886	46.551	1.00	27.86
	3950	CD1	LEU	B	917	35.492	22.792	45.701	1.00	32.98
	3951	CD2	LEU	B	917	33.750	24.346	46.572	1.00	37.82
50	3952	N	PRO	B	918	32.711	19.247	47.585	1.00	21.61
	3953	CA	PRO	B	918	32.919	18.490	48.822	1.00	26.49
	3954	C	PRO	B	918	33.838	17.292	48.586	1.00	24.53
55	3955	O	PRO	B	918	34.769	17.037	49.354	1.00	24.08
	3956	CB	PRO	B	918	31.498	18.053	49.194	1.00	25.82
	3957	CG	PRO	B	918	30.659	19.178	48.629	1.00	27.24
55	3958	CD	PRO	B	918	31.276	19.281	47.251	1.00	24.22
	3959	N	LYS	B	919	33.567	16.567	47.509	1.00	23.53
	3960	CA	LYS	B	919	34.339	15.381	47.159	1.00	26.07
	3961	C	LYS	B	919	35.811	15.729	46.938	1.00	23.29

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
3962	O	LYS	B	919	36.712	14.988	47.352	1.00	24.01
3963	CB	LYS	B	919	33.756	14.738	45.898	1.00	29.21
3964	CG	LYS	B	919	34.393	13.393	45.544	1.00	35.47
3965	CD	LYS	B	919	33.972	12.944	44.145	1.00	43.92
3966	CE	LYS	B	919	32.471	12.899	43.995	1.00	47.04
3967	NZ	LYS	B	919	32.081	12.653	42.573	1.00	55.56
3968	N	ILE	B	920	36.058	16.857	46.281	1.00	21.17
3969	CA	ILE	B	920	37.423	17.312	46.022	1.00	24.61
3970	C	ILE	B	920	38.167	17.663	47.320	1.00	26.60
3971	O	ILE	B	920	39.315	17.264	47.506	1.00	30.19
3972	CB	ILE	B	920	37.430	18.561	45.091	1.00	22.46
3973	CG1	ILE	B	920	37.000	18.162	43.681	1.00	26.76
3974	CG2	ILE	B	920	38.824	19.186	45.042	1.00	28.46
3975	CD1	ILE	B	920	36.707	19.354	42.795	1.00	29.32
3976	N	LEU	B	921	37.515	18.396	48.214	1.00	26.87
3977	CA	LEU	B	921	38.147	18.790	49.473	1.00	31.04
3978	C	LEU	B	921	38.414	17.603	50.375	1.00	30.07
3979	O	LEU	B	921	39.377	17.604	51.141	1.00	33.85
3980	CB	LEU	B	921	37.273	19.809	50.223	1.00	28.75
3981	CG	LEU	B	921	37.402	21.287	49.868	1.00	31.61
3982	CD1	LEU	B	921	36.346	22.078	50.621	1.00	31.82
3983	CD2	LEU	B	921	38.809	21.784	50.244	1.00	28.69
3984	N	ALA	B	922	37.570	16.579	50.280	1.00	28.13
3985	CA	ALA	B	922	37.735	15.389	51.108	1.00	28.58
3986	C	ALA	B	922	38.824	14.481	50.571	1.00	30.58
3987	O	ALA	B	922	39.070	13.418	51.125	1.00	32.70
3988	CB	ALA	B	922	36.433	14.626	51.185	1.00	28.32
3989	N	GLY	B	923	39.450	14.896	49.477	1.00	28.46
3990	CA	GLY	B	923	40.503	14.101	48.863	1.00	30.11
3991	C	GLY	B	923	39.990	12.843	48.197	1.00	29.47
3992	O	GLY	B	923	40.736	11.881	48.014	1.00	33.11
3993	N	MET	B	924	38.719	12.827	47.825	1.00	27.25
3994	CA	MET	B	924	38.156	11.635	47.202	1.00	28.82
3995	C	MET	B	924	38.222	11.681	45.680	1.00	30.78
3996	O	MET	B	924	37.290	11.270	44.993	1.00	27.46
3997	CB	MET	B	924	36.720	11.416	47.688	1.00	30.45
3998	CG	MET	B	924	36.664	11.091	49.176	1.00	35.29

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	3999	SD	MET	B	924	37.558	9.556	49.557	1.00	43.72
	4000	CE	MET	B	924	37.438	9.477	51.374	1.00	47.71
	4001	N	VAL	B	925	39.358	12.173	45.186	1.00	29.26
10	4002	CA	VAL	B	925	39.670	12.280	43.763	1.00	28.51
	4003	C	VAL	B	925	41.164	11.985	43.652	1.00	30.21
	4004	O	VAL	B	925	41.843	11.802	44.661	1.00	29.32
15	4005	CB	VAL	B	925	39.407	13.709	43.208	1.00	23.55
	4006	CG1	VAL	B	925	37.928	14.070	43.363	1.00	29.41
	4007	CG2	VAL	B	925	40.300	14.720	43.912	1.00	27.96
20	4008	N	LYS	B	926	41.687	11.946	42.437	1.00	29.24
	4009	CA	LYS	B	926	43.102	11.665	42.270	1.00	31.24
	4010	C	LYS	B	926	43.886	12.774	41.590	1.00	31.61
25	4011	O	LYS	B	926	43.894	12.902	40.364	1.00	27.27
	4012	CB	LYS	B	926	43.296	10.350	41.514	1.00	33.46
	4013	CG	LYS	B	926	44.744	10.011	41.236	1.00	39.59
30	4014	CD	LYS	B	926	44.880	8.556	40.803	1.00	46.42
	4015	CE	LYS	B	926	43.990	8.236	39.618	1.00	52.50
	4016	NZ	LYS	B	926	44.036	6.792	39.270	1.00	54.88
35	4017	N	PRO	B	927	44.523	13.628	42.394	1.00	30.89
	4018	CA	PRO	B	927	45.314	14.714	41.836	1.00	31.60
	4019	C	PRO	B	927	46.506	14.074	41.149	1.00	36.21
40	4020	O	PRO	B	927	47.058	13.088	41.639	1.00	32.44
	4021	CB	PRO	B	927	45.704	15.511	43.078	1.00	38.96
	4022	CG	PRO	B	927	45.811	14.413	44.131	1.00	38.64
45	4023	CD	PRO	B	927	44.507	13.713	43.864	1.00	33.53
	4024	N	LEU	B	928	46.886	14.609	40.000	1.00	33.51
	4025	CA	LEU	B	928	48.022	14.056	39.280	1.00	36.50
50	4026	C	LEU	B	928	49.230	14.937	39.545	1.00	38.84
	4027	O	LEU	B	928	49.217	16.135	39.276	1.00	41.78
	4028	CB	LEU	B	928	47.716	13.980	37.786	1.00	29.72
55	4029	CG	LEU	B	928	46.444	13.187	37.476	1.00	29.00
	4030	CD1	LEU	B	928	46.220	13.130	35.965	1.00	29.19
	4031	CD2	LEU	B	928	46.554	11.788	38.059	1.00	32.16
55	4032	N	LEU	B	929	50.270	14.334	40.101	1.00	35.29
	4033	CA	LEU	B	929	51.479	15.070	40.416	1.00	34.92
	4034	C	LEU	B	929	52.582	14.697	39.446	1.00	32.09
	4035	O	LEU	B	929	52.660	13.562	38.979	1.00	31.61

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	4036	CB	LEU	B	929	51.921	14.753	41.848	1.00	37.92
	4037	CG	LEU	B	929	51.014	15.258	42.970	1.00	40.28
	4038	CD1	LEU	B	929	51.465	14.689	44.295	1.00	44.21
10	4039	CD2	LEU	B	929	51.055	16.782	42.992	1.00	46.14
	4040	N	PHE	B	930	53.425	15.666	39.134	1.00	33.50
	4041	CA	PHE	B	930	54.534	15.426	38.235	1.00	37.57
15	4042	C	PHE	B	930	55.723	14.904	39.021	1.00	38.45
	4043	O	PHE	B	930	56.527	14.133	38.499	1.00	37.59
	4044	CB	PHE	B	930	54.929	16.710	37.515	1.00	36.92
20	4045	CG	PHE	B	930	53.861	17.252	36.624	1.00	36.88
	4046	CD1	PHE	B	930	52.880	18.103	37.123	1.00	34.19
	4047	CD2	PHE	B	930	53.817	16.887	35.281	1.00	41.45
25	4048	CE1	PHE	B	930	51.869	18.587	36.286	1.00	44.09
	4049	CE2	PHE	B	930	52.810	17.364	34.440	1.00	42.91
	4050	CZ	PHE	B	930	51.838	18.213	34.943	1.00	39.56
30	4051	N	HIS	B	931	55.803	15.311	40.285	1.00	36.07
	4052	CA	HIS	B	931	56.903	14.917	41.149	1.00	41.47
	4053	C	HIS	B	931	56.445	14.260	42.446	1.00	41.27
35	4054	O	HIS	B	931	55.401	14.697	42.972	1.00	45.00
	4055	CB	HIS	B	931	57.750	16.151	41.448	1.00	40.17
	4056	CG	HIS	B	931	58.212	16.864	40.215	1.00	48.97
40	4057	ND1	HIS	B	931	58.951	16.244	39.230	1.00	44.03
	4058	CD2	HIS	B	931	58.025	18.140	39.798	1.00	47.89
	4059	CE1	HIS	B	931	59.199	17.106	38.260	1.00	49.04
45	4060	NE2	HIS	B	931	58.650	18.264	38.581	1.00	50.90
	4061		HIS	B	931					
	4062	C1	STR	B	2	36.722	34.750	39.821	1.00	23.01
50	4063	C2	STR	B	2	37.383	34.885	38.411	1.00	30.18
	4064	C3	STR	B	2	38.878	35.052	38.581	1.00	29.08
	4065	O3	STR	B	2	39.501	35.761	37.778	1.00	35.44
55	4066	C4	STR	B	2	39.577	34.319	39.647	1.00	26.40
	4067	C5	STR	B	2	38.911	33.608	40.559	1.00	25.48
	4068	C6	STR	B	2	39.700	32.787	41.592	1.00	26.28
55	4069	C7	STR	B	2	39.171	32.980	43.035	1.00	22.37
	4070	C8	STR	B	2	37.627	32.810	43.155	1.00	23.98
	4071	C9	STR	B	2	36.932	33.817	42.168	1.00	20.64
	4072	C10	STR	B	2	37.329	33.590	40.661	1.00	20.19

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	4073	C11	STR	B	2	35.390	33.811	42.356	1.00	21.87
	4074	C12	STR	B	2	34.970	34.064	43.833	1.00	22.64
	4075	C13	STR	B	2	35.601	33.021	44.767	1.00	22.97
10	4076	C14	STR	B	2	37.164	33.157	44.578	1.00	24.84
	4077	C15	STR	B	2	37.755	32.350	45.755	1.00	27.19
	4078	C16	STR	B	2	36.767	32.674	46.938	1.00	28.64
15	4079	C17	STR	B	2	35.529	33.364	46.288	1.00	24.63
	4080	C18	STR	B	2	35.053	31.558	44.475	1.00	18.18
	4081	C19	STR	B	2	36.852	32.203	40.113	1.00	24.00
20	4082	C20	STR	B	2	34.178	33.098	46.985	1.00	26.21
	4083	O20	STR	B	2	34.028	32.147	47.721	1.00	30.43
	4084	C21	STR	B	2	33.060	34.033	46.751	1.00	25.53
25	4085	O	HOH		1000	33.666	17.404	87.251	1.00	22.19
	4086	O	HOH		1001	27.991	7.945	79.484	1.00	25.72
	4087	O	HOH		1002	16.741	15.065	72.689	1.00	29.58
30	4088	O	HOH		1003	36.823	15.614	69.042	1.00	23.68
	4089	O	HOH		1004	23.313	7.474	68.146	1.00	21.10
	4090	O	HOH		1005	45.633	27.074	27.131	1.00	31.65
35	4091	O	HOH		1006	37.862	19.992	22.137	1.00	22.34
	4092	O	HOH		1007	30.655	16.369	46.065	1.00	32.92
	4093	O	HOH		1008	27.171	36.648	41.698	1.00	25.15
40	4094	O	HOH		1009	44.296	28.506	25.056	1.00	24.87
	4095	O	HOH		1010	17.917	6.774	69.155	1.00	22.62
	4096	O	HOH		1011	37.660	29.818	22.972	1.00	27.17
45	4097	O	HOH		1012	37.688	23.686	40.855	1.00	27.87
	4098	O	HOH		1013	38.419	38.595	33.456	1.00	25.90
	4099	O	HOH		1014	30.427	9.090	51.398	1.00	29.15
50	4100	O	HOH		1015	58.710	17.046	23.597	1.00	27.03
	4101	O	HOH		1016	33.659	21.949	41.759	1.00	25.64
	4102	O	HOH		1017	32.808	13.290	64.116	1.00	28.14
55	4103	O	HOH		1018	10.078	12.182	57.163	1.00	32.35
	4104	O	HOH		1019	42.113	19.486	38.248	1.00	34.91
	4105	O	HOH		1020	41.094	18.002	36.209	1.00	26.81
55	4106	O	HOH		1021	30.979	15.363	63.422	1.00	28.79
	4107	O	HOH		1022	36.936	29.095	20.508	1.00	35.94
	4108	O	HOH		1023	40.497	23.491	40.659	1.00	23.11
	4109	O	HOH		1024	33.929	24.678	57.710	1.00	38.13

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	4110	O	HOH		1025	40.676	33.721	35.327	1.00	27.89
	4111	O	HOH		1026	40.680	28.650	53.024	1.00	33.04
	4112	O	HOH		1027	36.369	13.680	67.537	1.00	39.82
10	4113	O	HOH		1028	34.722	-5.251	80.392	1.00	32.81
	4114	O	HOH		1029	39.676	-3.503	86.330	1.00	36.01
	4115	O	HOH		1030	27.842	22.939	85.773	1.00	44.76
15	4116	O	HOH		1031	62.824	21.691	26.549	1.00	33.63
	4117	O	HOH		1032	16.427	-9.397	69.013	1.00	54.60
	4118	O	HOH		1033	36.222	14.728	63.426	1.00	51.82
20	4119	O	HOH		1034	43.556	21.247	45.108	1.00	29.39
	4120	O	HOH		1035	41.341	28.480	29.854	1.00	39.90
	4121	O	HOH		1036	51.585	48.214	48.363	1.00	30.49
25	4122	O	HOH		1037	22.687	4.551	72.387	1.00	36.18
	4123	O	HOH		1038	59.098	29.600	26.109	1.00	35.27
	4124	O	HOH		1039	55.684	35.659	26.274	1.00	42.35
30	4125	O	HOH		1040	31.061	18.050	82.280	1.00	21.99
	4126	O	HOH		1041	43.993	34.999	31.570	1.00	42.40
	4127	O	HOH		1042	12.626	17.393	61.026	1.00	33.69
35	4128	O	HOH		1043	42.167	23.707	63.170	1.00	51.66
	4129	O	HOH		1044	30.801	12.191	46.877	1.00	44.64
	4130	O	HOH		1045	48.081	49.753	47.195	1.00	35.43
40	4131	O	HOH		1046	30.363	26.610	56.223	1.00	32.27
	4132	O	HOH		1047	37.038	10.030	42.705	1.00	33.51
	4133	O	HOH		1048	23.093	13.225	81.215	1.00	42.96
45	4134	O	HOH		1049	33.482	20.462	20.296	1.00	36.45
	4135	O	HOH		1050	14.055	13.721	72.306	1.00	45.30
	4136	O	HOH		1051	28.811	43.105	52.857	1.00	63.86
50	4137	O	HOH		1052	47.646	34.627	52.909	1.00	36.00
	4138	O	HOH		1053	49.719	10.586	22.669	1.00	44.77
	4139	O	HOH		1054	43.185	10.462	60.207	1.00	48.26
55	4140	O	HOH		1055	27.182	6.289	49.610	1.00	52.31
	4141	O	HOH		1056	70.880	15.984	30.217	1.00	46.28
	4142	O	HOH		1057	35.128	4.502	35.039	1.00	51.40
	4143	O	HOH		1058	14.812	16.700	59.385	1.00	33.36
	4144	O	HOH		1059	46.460	34.689	40.532	1.00	34.71
	4145	O	HOH		1060	49.051	47.265	44.651	1.00	28.92
	4146	O	HOH		1061	45.167	51.194	41.329	1.00	46.31

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	4147	O	HOH		1062	29.592	-4.047	56.348	1.00	37.89
	4148	O	HOH		1063	32.458	36.767	54.252	1.00	63.27
	4149	O	HOH		1064	30.664	20.362	27.986	1.00	53.78
10	4150	O	HOH		1065	37.433	-13.669	66.706	1.00	65.87
	4151	O	HOH		1066	36.201	30.984	24.993	1.00	38.56
	4152	O	HOH		1067	46.351	13.151	75.804	1.00	55.39
15	4153	O	HOH		1068	33.456	12.303	40.428	1.00	58.95
	4154	O	HOH		1069	28.321	22.637	27.122	1.00	47.82
	4155	O	HOH		1070	40.552	14.140	55.956	1.00	53.39
20	4156	O	HOH		1071	26.098	12.641	88.207	1.00	61.83
	4157	O	HOH		1072	48.503	17.493	34.436	1.00	48.80
	4158	O	HOH		1073	42.177	48.877	43.220	1.00	27.83
25	4159	O	HOH		1074	38.062	47.031	49.044	1.00	44.21
	4160	O	HOH		1075	14.659	30.053	47.390	1.00	50.38
	4161	O	HOH		1076	23.348	29.500	45.003	1.00	31.93
30	4162	O	HOH		1077	17.005	32.707	54.248	1.00	54.07
	4163	O	HOH		1078	13.257	10.576	47.601	1.00	41.84
	4164	O	HOH		1079	30.618	-5.578	58.841	1.00	41.51
35	4165	O	HOH		1080	36.612	5.182	88.679	1.00	30.35
	4166	O	HOH		1081	35.761	31.204	55.444	1.00	49.87
	4167	O	HOH		1082	32.381	16.046	22.635	1.00	37.44
40	4168	O	HOH		1083	43.620	28.101	82.401	1.00	54.55
	4169	O	HOH		1084	8.058	8.892	73.013	1.00	55.15
	4170	O	HOH		1085	35.421	-7.443	88.230	1.00	49.25
45	4171	O	HOH		1086	27.342	7.972	45.641	1.00	50.17
	4172	O	HOH		1087	30.122	26.584	24.720	1.00	34.71
	4173	O	HOH		1088	26.449	11.806	48.387	1.00	51.75
50	4174	O	HOH		1089	16.902	21.688	55.310	1.00	35.02
	4175	O	HOH		1090	39.032	18.772	82.856	1.00	38.44
	4176	O	HOH		1091	33.889	-4.827	60.832	1.00	48.06
55	4177	O	HOH		1092	52.975	40.371	51.817	1.00	61.64
	4178	O	HOH		1093	27.906	51.315	40.663	1.00	46.27
	4179	O	HOH		1094	42.167	18.770	42.670	1.00	58.14
55	4180	O	HOH		1095	23.080	39.080	43.811	1.00	64.06
	4181	O	HOH		1096	34.247	25.343	19.682	1.00	42.03
	4182	O	HOH		1097	40.472	41.737	55.433	1.00	44.89
	4183	O	HOH		1098	56.942	34.297	20.120	1.00	58.67

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TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM	
5	4184	O	HOH		1099	66.188	19.205	40.041	1.00	58.84
	4185	O	HOH		1100	36.630	11.860	62.910	1.00	37.72
	4186	O	HOH		1101	26.825	18.353	46.932	1.00	40.45
10	4187	O	HOH		1102	22.250	32.330	37.131	1.00	53.43
	4188	O	HOH		1103	57.886	40.754	42.618	1.00	42.31
	4189	O	HOH		1104	46.731	16.884	21.013	1.00	59.18
15	4190	O	HOH		1105	25.096	10.702	74.366	1.00	49.26
	4191	O	HOH		1106	41.831	26.244	69.694	1.00	50.01
	4192	O	HOH		1107	24.979	14.834	86.465	1.00	58.25
20	4193	O	HOH		1108	42.044	-18.293	88.405	1.00	53.84
	4194	O	HOH		1109	60.868	31.903	29.340	1.00	56.15
	4195	O	HOH		1110	47.828	8.529	78.005	1.00	57.38
25	4196	O	HOH		1111	30.517	10.898	25.227	1.00	43.12
	4197	O	HOH		1112	26.673	45.793	49.522	1.00	42.53
	4198	O	HOH		1113	40.395	7.287	85.552	1.00	34.61
30	4199	O	HOH		1114	36.002	50.942	48.176	1.00	55.29
	4200	O	HOH		1115	15.517	1.041	72.791	1.00	32.07
	4201	O	HOH		1116	24.858	15.134	26.431	1.00	49.39
35	4202	O	HOH		1117	31.562	34.334	28.869	1.00	36.46
	4203	O	HOH		1118	35.859	-12.062	72.482	1.00	54.03
	4204	O	HOH		1119	57.184	43.582	38.922	1.00	42.30
40	4205	O	HOH		1120	20.561	-8.563	70.577	1.00	60.48
	4206	O	HOH		1121	39.714	-9.373	72.709	1.00	42.35
	4207	O	HOH		1122	29.084	21.194	77.543	1.00	55.53
45	4208	O	HOH		1123	26.622	15.926	35.036	1.00	49.36
	4209	O	HOH		1124	21.471	9.364	71.434	1.00	41.52
	4210	O	HOH		1125	30.481	19.290	62.284	1.00	32.09
50	4211	O	HOH		1126	35.637	11.560	67.233	1.00	46.34
	4212	O	HOH		1127	11.013	0.808	62.566	1.00	41.40
	4213	O	HOH		1128	33.112	34.801	52.664	1.00	42.33
55	4214	O	HOH		1129	17.395	15.298	75.306	1.00	38.43
	4215	O	HOH		1130	12.781	11.039	72.132	1.00	36.36
	4216	O	HOH		1131	29.971	28.037	26.998	1.00	37.72
55	4217	O	HOH		1132	18.569	-10.048	69.689	1.00	49.58
	4218	O	HOH		1133	41.228	21.065	46.519	1.00	37.30
	4219	O	HOH		1134	37.135	24.743	63.591	1.00	49.04
	4220	O	HOH		1135	27.047	1.783	63.648	1.00	31.46

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG										
	ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
5	4221	O	HOH		1136	7.627	13.172	67.948	1.00	47.51
	4222	O	HOH		1137	30.244	21.919	32.671	1.00	51.61
	4223	O	HOH		1138	23.072	31.139	55.222	1.00	40.35
10	4224	O	HOH		1139	18.856	13.261	76.752	1.00	51.54
	4225	O	HOH		1140	14.629	17.453	71.521	1.00	44.61
	4226	O	HOH		1141	30.127	7.542	77.644	1.00	39.23
15	4227	O	HOH		1142	29.410	10.319	49.169	1.00	47.59
	4228	O	HOH		1143	52.667	17.385	21.488	1.00	33.48
	4229	O	HOH		1144	24.791	30.379	57.499	1.00	50.29
20	4230	O	HOH		1145	33.515	32.303	54.663	1.00	60.00
	4231	O	HOH		1146	43.670	11.568	23.068	1.00	42.60
	4232	O	HOH		1147	22.577	-0.615	76.831	1.00	51.25
25	4233	O	HOH		1148	32.288	40.493	29.506	1.00	44.45
	4234	O	HOH		1149	38.587	13.656	83.878	1.00	50.82
	4235	O	HOH		1150	49.160	49.467	49.792	1.00	43.40
30	4236	O	HOH		1151	36.423	9.754	65.069	1.00	50.09
	4237	O	HOH		1152	41.806	7.306	67.548	1.00	31.99
	4238	O	HOH		1153	20.865	5.502	75.530	1.00	53.88
35	4239	O	HOH		1154	26.670	47.493	47.589	1.00	51.95
	4240	O	HOH		1155	58.759	25.881	41.102	1.00	51.36
	4241	O	HOH		1156	22.627	35.482	48.933	1.00	49.41
40	4242	O	HOH		1157	29.902	41.245	33.231	1.00	47.09
	4243	O	HOH		1158	42.020	38.368	56.303	1.00	54.13
	4244	O	HOH		1159	42.067	18.958	48.188	1.00	41.24
45	4245	O	HOH		1160	50.498	28.461	49.894	1.00	58.63
	4246	O	HOH		1161	19.503	21.644	46.170	1.00	47.41
	4247	O	HOH		1162	23.864	30.453	31.232	1.00	50.37
50	4248	O	HOH		1163	33.055	31.002	70.386	1.00	45.87
	4249	O	HOH		1164	69.219	22.617	25.319	1.00	54.13
	4250	O	HOH		1165	26.984	34.792	32.747	1.00	50.24
55	4251	O	HOH		1166	18.904	22.434	40.238	1.00	55.76
	4252	O	HOH		1167	38.572	18.970	85.692	1.00	51.19
	4253	O	HOH		1168	55.921	7.586	67.043	1.00	56.10
55	4254	O	HOH		1169	60.815	24.101	20.645	1.00	43.40
	4255	O	HOH		1170	36.032	13.461	58.415	1.00	36.46
	4256	O	HOH		1171	42.102	18.389	50.609	1.00	50.87
	4257	O	HOH		1172	61.353	15.073	41.877	1.00	55.08

TABLE 10 (continued)

THREE-DIMENSIONAL COORDINATES OF PR IN COMPLEX WITH PG									
ATOM	ATOM TYPE	RESIDUE	#	X	Y	Z	OCC	B	ATOM
4258	O	HOH		1173	34.024	3.531	28.705	1.00	52.74
4259	O	HOH		1174	41.542	7.988	49.104	1.00	55.00
4260	O	HOH		1175	24.756	2.570	77.011	1.00	53.63
4261	O	HOH		1176	41.140	5.822	60.200	1.00	39.74
4262	O	HOH		1177	9.209	2.894	61.066	1.00	48.67
4263	O	HOH		1178	37.046	11.589	60.375	1.00	40.88
4264	O	HOH		1179	35.350	29.505	79.245	1.00	38.37

TABLE 11

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
1	CB	THR	729	-19.756	38.320	19.110
2	C	THR	729	-18.114	38.275	17.211
3	O	THR	729	-16.947	37.873	17.214
4	N	THR	729	-18.598	36.174	18.360
5	CA	THR	729	-19.213	37.506	17.945
6	OG1	THR	729	-20.818	37.625	19.751
7	CG2	THR	729	-20.352	39.701	18.762
8	N	ILE	730	-18.503	39.394	16.608
9	CA	ILE	730	-17.623	40.222	15.789
10	CB	ILE	730	-18.297	41.571	15.469
11	C	ILE	730	-16.196	40.504	16.195
12	O	ILE	730	-15.740	40.220	17.294
13	CG2	ILE	730	-17.440	42.465	14.521
14	CG1	ILE	730	-19.731	41.454	14.861
15	CD1	ILE	730	-20.557	42.757	14.828
16	N	SER	731	-15.505	41.060	15.220
17	CA	SER	731	-14.134	41.446	15.326
18	CB	SER	731	-13.299	40.445	16.166
19	C	SER	731	-13.634	41.573	13.874
20	O	SER	731	-14.280	41.111	12.934
21	OG	SER	731	-13.117	39.185	15.512
22	N	ARG	732	-12.466	42.196	13.695
23	CA	ARG	732	-11.890	42.630	14.953
24	CB	ARG	732	-10.516	43.184	14.585
25	C	ARG	732	-12.607	43.506	15.952

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	26	O	ARG	732	-13.827	43.743	15.969
	27	CG	ARG	732	-10.508	44.628	14.011
10	28	CD	ARG	732	-9.081	45.148	13.769
	29	NE	ARG	732	-9.137	46.534	13.219
	30	CZ	ARG	732	-8.082	47.277	12.899
	31	NH1	ARG	732	-8.288	48.469	12.437
15	32	NH2	ARG	732	-6.849	46.871	13.023
	33	N	ALA	733	-11.742	43.858	16.871
	34	CA	ALA	733	-12.003	44.602	18.044
20	35	CB	ALA	733	-10.933	45.657	18.148
	36	C	ALA	733	-13.363	45.135	18.293
	37	O	ALA	733	-13.652	46.285	18.018
	38	N	LEU	734	-14.245	44.261	18.739
25	39	CA	LEU	734	-15.501	44.789	19.161
	40	CB	LEU	734	-16.704	44.008	18.666
	41	CG	LEU	734	-17.555	45.126	18.047
30	42	CD1	LEU	734	-18.950	44.631	17.803
	43	CD2	LEU	734	-17.589	46.355	18.973
	44	C	LEU	734	-15.240	44.562	20.626
	45	O	LEU	734	-16.127	44.626	21.465
35	46	N	THR	735	-13.962	44.302	20.897
	47	CA	THR	735	-13.428	44.048	22.224
	48	CB	THR	735	-13.995	42.763	22.803
40	49	OG1	THR	735	-14.494	41.807	21.860
	50	CG2	THR	735	-15.075	43.091	23.820
	51	C	THR	735	-11.918	43.943	22.076
	52	O	THR	735	-11.364	42.855	21.905
45	53	N	PRO	736	-11.241	45.088	22.203
	54	CD	PRO	736	-11.886	45.982	23.170
	55	CA	PRO	736	-9.820	45.423	22.111
50	56	CB	PRO	736	-9.750	46.869	22.596
	57	CG	PRO	736	-11.131	47.234	22.999
	58	C	PRO	736	-8.819	44.559	22.827
	59	O	PRO	736	-9.060	44.008	23.899
55	60	N	SER	737	-7.645	44.523	22.226
	61	CA	SER	737	-6.573	43.708	22.713

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
62	CB	SER	737	-6.182	42.760	21.638
63	C	SER	737	-5.375	44.525	23.067
64	O	SER	737	-5.269	45.692	22.693
65	OG	SER	737	-7.176	41.760	21.389
66	N	PRO	738	-4.443	43.914	23.765
67	CA	PRO	738	-3.306	44.709	24.076
68	CB	PRO	738	-2.291	43.940	24.906
69	C	PRO	738	-2.684	45.293	22.811
70	O	PRO	738	-2.438	46.498	22.731
71	CG	PRO	738	-2.473	42.521	24.341
72	CD	PRO	738	-3.991	42.390	24.175
73	N	VAL	739	-2.500	44.447	21.804
74	CA	VAL	739	-1.889	44.833	20.541
75	CB	VAL	739	-1.508	43.576	19.786
76	CG1	VAL	739	-2.772	42.871	19.326
77	CG2	VAL	739	-0.607	43.918	18.640
78	C	VAL	739	-2.741	45.703	19.604
79	O	VAL	739	-2.250	46.235	18.608
80	N	MET	740	-4.019	45.833	19.923
81	CA	MET	740	-4.941	46.603	19.100
82	CB	MET	740	-6.349	46.084	19.336
83	C	MET	740	-4.875	48.043	19.513
84	O	MET	740	-4.947	48.972	18.706
85	CG	MET	740	-6.600	44.615	18.934
86	SD	MET	740	-8.364	44.257	19.004
87	CE	MET	740	-8.277	42.465	18.887
88	N	VAL	741	-4.766	48.181	20.818
89	CA	VAL	741	-4.694	49.442	21.487
90	CB	VAL	741	-4.802	49.170	22.971
91	C	VAL	741	-3.357	50.057	21.149
92	O	VAL	741	-3.223	51.269	20.958
93	CG1	VAL	741	-6.167	48.580	23.404
94	CG2	VAL	741	-4.562	50.382	23.914
95	N	LEU	742	-2.362	49.190	21.059
96	CA	LEU	742	-1.019	49.623	20.753
97	CB	LEU	742	-0.084	48.427	20.896

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	98	CG	LEU	742	1.010	48.630	21.951
	99	CD1	LEU	742	0.433	49.160	23.240
10	100	CD2	LEU	742	1.711	47.316	22.185
	101	C	LEU	742	-0.929	50.237	19.357
	102	O	LEU	742	-0.092	51.104	19.094
	103	N	GLU	743	-1.833	49.795	18.487
15	104	CA	GLU	743	-1.904	50.219	17.097
	105	CB	GLU	743	-2.756	49.212	16.320
	106	CG	GLU	743	-2.136	48.796	15.007
20	107	CD	GLU	743	-2.570	47.415	14.514
	108	OE1	GLU	743	-2.934	46.529	15.329
	109	OE2	GLU	743	-2.513	47.214	13.284
	110	C	GLU	743	-2.452	51.624	16.871
25	111	O	GLU	743	-1.996	52.337	15.977
	112	N	ASN	744	-3.423	52.016	17.680
	113	CA	ASN	744	-4.044	53.316	17.530
30	114	CB	ASN	744	-5.471	53.284	18.055
	115	C	ASN	744	-3.287	54.388	18.276
	116	O	ASN	744	-3.311	55.556	17.890
	117	CG	ASN	744	-6.417	52.253	17.431
35	118	OD1	ASN	744	-6.684	51.196	17.983
	119	ND2	ASN	744	-6.937	52.503	16.259
	120	N	ILE	745	-2.614	54.006	19.356
40	121	CA	ILE	745	-1.896	55.023	20.098
	122	CB	ILE	745	-1.765	54.673	21.610
	123	CG2	ILE	745	-3.046	54.028	22.106
	124	CG1	ILE	745	-0.582	53.744	21.859
45	125	CD1	ILE	745	-0.178	53.699	23.317
	126	C	ILE	745	-0.524	55.320	19.509
	127	O	ILE	745	0.161	56.226	19.973
50	128	N	GLU	746	-0.132	54.573	18.479
	129	CA	GLU	746	1.167	54.785	17.826
	130	CB	GLU	746	1.409	53.704	16.753
	131	CG	GLU	746	2.741	53.793	15.984
55	132	CD	GLU	746	3.990	53.653	16.855
	133	OE1	GLU	746	4.303	52.528	17.298

TABLE 11 (continued)

TABLE 11 (continued)							
THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
5	134	OE2	GLU	746	4.670	54.674	17.093
	135	C	GLU	746	1.160	56.185	17.203
	136	O	GLU	746	0.281	56.514	16.399
10	137	N	PRO	747	2.114	57.042	17.597
	138	CD	PRO	747	3.001	57.025	18.773
	139	CA	PRO	747	2.080	58.369	16.985
15	140	CB	PRO	747	3.240	59.122	17.655
	141	CG	PRO	747	4.002	58.090	18.432
	142	C	PRO	747	2.211	58.315	15.484
	143	O	PRO	747	2.743	57.347	14.931
20	144	N	GLU	748	1.691	59.331	14.813
	145	CA	GLU	748	1.833	59.328	13.380
	146	CB	GLU	748	0.511	59.651	12.673
25	147	CG	GLU	748	-0.106	61.009	12.712
	148	CD	GLU	748	-1.176	61.042	11.636
	149	OE1	GLU	748	-2.016	60.110	11.627
	150	OE2	GLU	748	-1.169	61.956	10.785
30	151	C	GLU	748	3.010	60.222	13.010
	152	O	GLU	748	3.380	61.117	13.764
	153	N	ILE	749	3.618	59.939	11.860
35	154	CA	ILE	749	4.850	60.602	11.416
	155	CB	ILE	749	5.212	59.980	10.004
	156	C	ILE	749	5.059	62.115	11.226
	157	O	ILE	749	4.357	62.768	10.453
40	158	CG2	ILE	749	5.462	58.447	10.077
	159	CG1	ILE	749	4.309	60.289	8.765
	160	CD1	ILE	749	2.804	59.971	8.865
45	161	N	VAL	750	6.091	62.639	11.893
	162	CA	VAL	750	6.453	64.069	11.856
	163	CB	VAL	750	6.926	64.489	13.295
	164	C	VAL	750	7.513	64.559	10.849
50	165	O	VAL	750	8.707	64.280	11.013
	166	CG1	VAL	750	5.820	64.279	14.360
	167	CG2	VAL	750	7.395	65.961	13.399
55	168	N	TYR	751	7.070	65.321	9.841
	169	CA	TYR	751	7.956	65.903	8.814

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	170	CB	TYR	751	7.131	66.540	7.688
	171	CG	TYR	751	6.395	65.498	6.878
10	172	CD1	TYR	751	5.170	64.989	7.305
	173	CE1	TYR	751	4.564	63.915	6.641
	174	CD2	TYR	751	6.988	64.921	5.756
	175	CE2	TYR	751	6.399	63.851	5.089
15	176	CZ	TYR	751	5.187	63.350	5.537
	177	OH	TYR	751	4.593	62.295	4.880
	178	C	TYR	751	8.851	66.939	9.489
20	179	O	TYR	751	8.486	67.464	10.534
	180	N	ALA	752	9.999	67.259	8.893
	181	CA	ALA	752	10.931	68.180	9.550
	182	CB	ALA	752	12.356	67.636	9.405
25	183	C	ALA	752	10.942	69.673	9.246
	184	O	ALA	752	11.638	70.420	9.935
	185	N	GLY	753	10.195	70.128	8.246
30	186	CA	GLY	753	10.213	71.550	7.933
	187	C	GLY	753	11.621	71.989	7.557
	188	O	GLY	753	12.086	73.063	7.941
	189	N	TYR	754	12.309	71.142	6.812
35	190	CA	TYR	754	13.662	71.437	6.386
	191	CB	TYR	754	14.402	70.140	6.103
	192	CG	TYR	754	15.874	70.279	5.811
40	193	CD1	TYR	754	16.792	70.476	6.840
	194	CE1	TYR	754	18.162	70.466	6.595
	195	CD2	TYR	754	16.362	70.099	4.518
	196	CE2	TYR	754	17.724	70.090	4.263
45	197	CZ	TYR	754	18.618	70.268	5.309
	198	OH	TYR	754	19.972	70.240	5.048
	199	C	TYR	754	13.557	72.238	5.112
50	200	O	TYR	754	12.560	72.161	4.396
	201	N	ASP	755	14.576	73.024	4.822
	202	CA	ASP	755	14.548	73.803	3.609
	203	CB	ASP	755	14.825	75.267	3.915
55	204	CG	ASP	755	14.947	76.086	2.669
	205	OD1	ASP	755	14.292	75.709	1.677

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
206	OD2	ASP	755	15.684	77.091	2.677
207	C	ASP	755	15.600	73.242	2.673
208	O	ASP	755	16.777	73.546	2.795
209	N	SER	756	15.179	72.412	1.730
210	CA	SER	756	16.139	71.822	0.812
211	CB	SER	756	15.731	70.385	0.440
212	OG	SER	756	14.414	70.273	-0.094
213	C	SER	756	16.338	72.672	-0.423
214	O	SER	756	17.007	72.262	-1.373
215	N	SER	757	15.754	73.858	-0.427
216	CA	SER	757	15.981	74.718	-1.564
217	CB	SER	757	14.974	75.867	-1.613
218	OG	SER	757	14.787	76.751	-0.529
219	C	SER	757	17.416	75.229	-1.427
220	O	SER	757	17.984	75.718	-2.385
221	N	LYS	758	18.018	75.104	-0.245
222	CA	LYS	758	19.410	75.542	-0.084
223	CB	LYS	758	19.569	76.631	1.022
224	C	LYS	758	20.317	74.345	0.233
225	O	LYS	758	19.879	73.368	0.846
226	CG	LYS	758	21.018	77.164	1.158
227	CD	LYS	758	21.225	78.187	2.279
228	CE	LYS	758	22.709	78.571	2.345
229	NZ	LYS	758	22.886	79.678	3.301
230	N	PRO	759	21.605	74.418	-0.156
231	CD	PRO	759	22.272	75.497	-0.900
232	CA	PRO	759	22.533	73.305	0.094
233	CB	PRO	759	23.747	73.665	-0.752
234	CG	PRO	759	23.733	75.132	-0.765
235	C	PRO	759	22.917	72.865	1.503
236	O	PRO	759	23.305	73.661	2.360
237	N	ASP	760	22.822	71.551	1.685
238	CA	ASP	760	23.121	70.877	2.939
239	CB	ASP	760	23.112	69.349	2.763
240	CG	ASP	760	21.888	68.816	2.030
241	OD1	ASP	760	20.960	69.573	1.668

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	242	OD2	ASP	760	21.879	67.589	1.818
	243	C	ASP	760	24.480	71.222	3.533
10	244	O	ASP	760	25.312	71.900	2.930
	245	N	THR	761	24.689	70.695	4.731
	246	CA	THR	761	25.915	70.844	5.482
	247	CB	THR	761	26.423	72.285	5.820
15	248	C	THR	761	25.635	70.009	6.710
	249	O	THR	761	24.476	69.815	7.079
	250	OG1	THR	761	27.630	72.232	6.576
20	251	CG2	THR	761	25.418	73.203	6.527
	252	N	ALA	762	26.684	69.510	7.336
	253	CA	ALA	762	26.498	68.676	8.506
	254	CB	ALA	762	27.840	68.117	9.005
25	255	C	ALA	762	25.771	69.331	9.673
	256	O	ALA	762	24.899	68.692	10.267
	257	N	GLU	763	26.115	70.581	10.011
30	258	CA	GLU	763	25.476	71.272	11.144
	259	CB	GLU	763	26.194	72.592	11.546
	260	C	GLU	763	24.007	71.553	10.871
	261	O	GLU	763	23.157	71.402	11.744
35	262	CG	GLU	763	26.307	73.719	10.479
	263	CD	GLU	763	25.265	74.895	10.561
	264	OE1	GLU	763	24.497	74.906	11.528
40	265	OE2	GLU	763	25.344	75.705	9.631
	266	N	ASN	764	23.716	71.939	9.645
	267	CA	ASN	764	22.360	72.239	9.245
	268	CB	ASN	764	22.372	72.902	7.845
45	269	C	ASN	764	21.486	71.002	9.189
	270	O	ASN	764	20.262	71.061	9.294
	271	CG	ASN	764	20.995	73.387	7.376
50	272	OD1	ASN	764	20.215	73.953	8.123
	273	ND2	ASN	764	20.735	73.180	6.002
	274	N	LEU	765	22.127	69.872	8.974
	275	CA	LEU	765	21.391	68.644	8.848
55	276	CB	LEU	765	22.223	67.683	7.963
	277	C	LEU	765	21.024	68.015	10.158

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
5	278	O	LEU	765	20.024	67.298	10.275
	279	CG	LEU	765	21.499	66.430	7.442
	280	CD1	LEU	765	20.143	66.766	6.772
10	281	CD2	LEU	765	22.437	65.683	6.467
	282	N	LEU	766	21.877	68.222	11.136
	283	CA	LEU	766	21.567	67.619	12.386
15	284	CB	LEU	766	22.728	66.737	12.939
	285	C	LEU	766	21.005	68.605	13.352
	286	O	LEU	766	20.877	68.318	14.530
	287	CG	LEU	766	23.913	67.344	13.722
20	288	CD1	LEU	766	25.193	66.496	13.527
	289	CD2	LEU	766	24.184	68.811	13.399
	290	N	SER	767	20.684	69.800	12.908
25	291	CA	SER	767	20.024	70.574	13.906
	292	CB	SER	767	20.276	72.095	13.791
	293	C	SER	767	18.550	70.269	13.691
	294	O	SER	767	17.829	69.980	14.640
30	295	OG	SER	767	19.523	72.823	14.751
	296	N	THR	768	18.110	70.288	12.437
	297	CA	THR	768	16.720	70.012	12.116
35	298	CB	THR	768	16.570	69.964	10.593
	299	OG1	THR	768	17.092	71.157	9.999
	300	CG2	THR	768	15.112	69.830	10.188
40	301	C	THR	768	16.319	68.674	12.738
	302	O	THR	768	15.155	68.460	13.145
	303	N	LEU	769	17.315	67.800	12.839
	304	CA	LEU	769	17.137	66.464	13.346
45	305	CB	LEU	769	18.395	65.722	12.955
	306	CG	LEU	769	18.165	64.572	11.949
	307	CD1	LEU	769	17.010	64.884	10.998
	308	CD2	LEU	769	19.424	64.310	11.136
50	309	C	LEU	769	16.906	66.514	14.857
	310	O	LEU	769	16.098	65.774	15.452
	311 1	N	ASN	770	17.642	67.402	15.485
55	312	CA	ASN	770	17.460	67.562	16.888
	313	CB	ASN	770	18.532	68.480	17.376

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	314	CG	ASN	770	19.775	67.729	17.672
	315	OD1	ASN	770	20.089	66.732	17.016
10	316	ND2	ASN	770	20.607	68.445	18.542
	317	C	ASN	770	16.073	68.135	17.052
	318	O	ASN	770	15.238	67.569	17.732
	319	N	ARG	771	15.825	69.267	16.420
15	320	CA	ARG	771	14.516	69.874	16.457
	321	CB	ARG	771	14.469	70.956	15.411
	322	CG	ARG	771	15.421	72.167	15.625
20	323	C	ARG	771	13.456	68.815	16.170
	324	O	ARG	771	12.379	68.841	16.763
	325	CD	ARG	771	15.508	73.114	14.406
	326	NE	ARG	771	14.248	73.390	13.674
25	327	CZ	ARG	771	14.132	73.721	12.336
	328	NH1	ARG	771	12.884	73.956	11.815
	329	NH2	ARG	771	15.225	73.819	11.507
30	330	N	LEU	772	13.735	67.891	15.253
	331	CA	LEU	772	12.746	66.848	15.013
	332	CB	LEU	772	13.098	65.965	13.804
	333	CG	LEU	772	11.863	65.253	13.219
35	334	CD1	LEU	772	12.216	63.962	12.506
	335	CD2	LEU	772	10.921	64.937	14.353
	336	C	LEU	772	12.792	66.025	16.305
40	337	O	LEU	772	11.797	65.443	16.737
	338	N	ALA	773	13.968	66.008	16.927
	339	CA	ALA	773	14.160	65.294	18.178
	340	C	ALA	773	13.152	65.700	19.236
45	341	O	ALA	773	12.378	64.862	19.695
	342	CB	ALA	773	15.616	65.518	18.624
	343	N	GLY	774	13.146	66.976	19.621
50	344	CA	GLY	774	12.204	67.432	20.625
	345	C	GLY	774	10.763	67.024	20.350
	346	O	GLY	774	10.122	66.392	21.188
	347	N	LYS	775	10.248	67.369	19.178
55	348	CA	LYS	775	8.868	67.045	18.855
	349	CB	LYS	775	8.525	67.530	17.445

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
350	CG	LYS	775	8.419	69.054	17.353
351	CD	LYS	775	7.791	69.503	16.016
352	C	LYS	775	8.539	65.569	19.005
353	O	LYS	775	7.517	65.206	19.591
354	CE	LYS	775	7.787	71.028	15.818
355	NZ	LYS	775	7.242	71.426	14.456
356	N	GLN	776	9.412	64.719	18.477
357	CA	GLN	776	9.214	63.279	18.555
358	CB	GLN	776	10.318	62.566	17.788
359	CG	GLN	776	9.887	61.973	16.466
360	CD	GLN	776	11.078	61.625	15.631
361	OE1	GLN	776	10.948	61.242	14.472
362	NE2	GLN	776	12.331	61.695	16.275
363	C	GLN	776	9.218	62.800	19.996
364	O	GLN	776	8.373	61.998	20.393
365	N	MET	777	10.182	63.283	20.770
366	CA	MET	777	10.298	62.919	22.176
367	CB	MET	777	11.478	63.747	22.759
368	C	MET	777	9.015	63.253	22.923
369	O	MET	777	8.505	62.443	23.702
370	CG	MET	777	11.739	63.416	24.216
371	SD	MET	777	11.922	61.626	24.254
372	CE	MET	777	11.174	61.295	25.852
373	N	ILE	778	8.508	64.461	22.687
374	CA	ILE	778	7.271	64.908	23.318
375	CB	ILE	778	6.941	66.366	22.911
376	CG2	ILE	778	5.432	66.624	22.997
377	CG1	ILE	778	7.725	67.325	23.820
378	CD1	ILE	778	8.335	68.525	23.116
379	C	ILE	778	6.161	63.965	22.902
380	O	ILE	778	5.392	63.509	23.735
381	N	GLN	779	6.088	63.655	21.621
382	CA	GLN	779	5.070	62.736	21.133
383	CB	GLN	779	5.125	62.293	19.652
384	C	GLN	779	5.123	61.425	21.925
385	O	GLN	779	4.083	60.818	22.219

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	386	CG	GLN	779	4.732	63.341	18.595
	387	CD	GLN	779	4.569	62.623	17.248
10	388	OE1	GLN	779	5.502	62.033	16.728
	389	NE2	GLN	779	3.274	62.678	16.676
	390	N	VAL	780	6.345	61.004	22.264
	391	CA	VAL	780	6.590	59.764	23.003
15	392	CB	VAL	780	8.113	59.380	23.122
	393	C	VAL	780	5.932	59.780	24.373
	394	O	VAL	780	5.427	58.760	24.842
20	395	CG1	VAL	780	8.564	58.449	21.970
	396	CG2	VAL	780	8.538	58.770	24.479
	397	N	VAL	781	5.951	60.945	25.014
	398	CA	VAL	781	5.346	61.101	26.324
25	399	CB	VAL	781	5.625	62.498	26.891
	400	CG1	VAL	781	5.016	62.620	28.253
	401	CG2	VAL	781	7.111	62.740	26.963
30	402	C	VAL	781	3.825	60.855	26.267
	403	O	VAL	781	3.306	60.031	27.019
	404	N	LYS	782	3.118	61.548	25.370
	405	CA	LYS	782	1.659	61.390	25.231
35	406	CB	LYS	782	1.118	62.386	24.204
	407	CG	LYS	782	-0.352	62.165	23.801
	408	CD	LYS	782	-0.801	63.198	22.762
40	409	CE	LYS	782	-0.465	64.627	23.229
	410	NZ	LYS	782	-0.605	65.690	22.152
	411	C	LYS	782	1.274	59.973	24.800
	412	O	LYS	782	0.106	59.571	24.861
45	413	N	TRP	783	2.281	59.238	24.351
	414	CA	TRP	783	2.152	57.862	23.881
	415	CB	TRP	783	3.212	57.595	22.816
50	416	CG	TRP	783	3.470	56.155	22.564
	417	CD2	TRP	783	4.588	55.392	23.026
	418	CE2	TRP	783	4.399	54.069	22.586
	419	CE3	TRP	783	5.723	55.696	23.794
55	420	CD1	TRP	783	2.677	55.293	21.869
	421	NE1	TRP	783	3.228	54.039	21.875

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
422	CZ2	TRP	783	5.317	53.047	22.855
423	CZ3	TRP	783	6.634	54.679	24.067
424	CH2	TRP	783	6.421	53.370	23.606
425	C	TRP	783	2.377	56.910	25.039
426	O	TRP	783	1.644	55.939	25.215
427	N	ALA	784	3.430	57.186	25.804
428	CA	ALA	784	3.785	56.365	26.948
429	CB	ALA	784	4.985	56.962	27.673
430	C	ALA	784	2.593	56.305	27.881
431	O	ALA	784	2.217	55.241	28.357
432	N	LYS	785	1.992	57.466	28.114
433	CA	LYS	785	0.847	57.573	28.992
434	CB	LYS	785	0.509	59.053	29.222
435	CG	LYS	785	1.737	59.940	29.510
436	CD	LYS	785	1.413	61.389	29.990
437	CE	LYS	785	0.003	61.884	29.609
438	NZ	LYS	785	-0.348	63.263	30.145
439	C	LYS	785	-0.381	56.817	28.479
440	O	LYS	785	-1.349	56.670	29.211
441	N	VAL	786	-0.367	56.328	27.242
442	CA	VAL	786	-1.532	55.592	26.746
443	CB	VAL	786	-1.855	55.995	25.312
444	C	VAL	786	-1.323	54.085	26.826
445	O	VAL	786	-2.267	53.307	26.643
446	CG1	VAL	786	-2.296	57.471	25.159
447	CG2	VAL	786	-2.951	55.162	24.592
448	N	LEU	787	-0.079	53.681	27.083
449	CA	LEU	787	0.257	52.268	27.214
450	CB	LEU	787	1.775	52.044	27.401
451	C	LEU	787	-0.470	51.832	28.467
452	O	LEU	787	-0.109	52.208	29.587
453	CG	LEU	787	2.734	52.584	26.306
454	CD1	LEU	787	4.178	52.168	26.617
455	CD2	LEU	787	2.350	52.109	24.895
456	N	PRO	788	-1.543	51.063	28.293
457	CD	PRO	788	-2.126	50.571	27.034

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	458	CA	PRO	788	-2.287	50.611	29.461
	459	CB	PRO	788	-3.126	49.444	28.917
10	460	CG	PRO	788	-2.658	49.248	27.445
	461	C	PRO	788	-1.346	50.207	30.603
	462	O	PRO	788	-0.498	49.331	30.431
	463	N	GLY	789	-1.469	50.871	31.751
15	464	CA	GLY	789	-0.628	50.533	32.889
	465	C	GLY	789	0.592	51.398	33.148
	466	O	GLY	789	1.087	51.477	34.273
20	467	N	PHE	790	1.106	52.057	32.125
	468	CA	PHE	790	2.271	52.877	32.357
	469	CB	PHE	790	2.789	53.462	31.052
	470	CG	PHE	790	3.949	54.379	31.239
25	471	CD1	PHE	790	5.220	53.870	31.479
	472	CD2	PHE	790	3.768	55.750	31.196
	473	CE1	PHE	790	6.300	54.717	31.695
30	474	CE2	PHE	790	4.840	56.612	31.410
	475	CZ	PHE	790	6.112	56.096	31.653
	476	C	PHE	790	1.972	54.015	33.328
	477	O	PHE	790	2.849	54.414	34.108
35	478	N	LYS	791	0.752	54.548	33.304
	479	CA	LYS	791	0.510	55.667	34.201
	480	CB	LYS	791	-0.334	56.759	33.530
40	481	CG	LYS	791	-1.744	56.478	33.055
	482	CD	LYS	791	-2.230	57.816	32.484
	483	C	LYS	791	0.026	55.391	35.608
	484	O	LYS	791	-0.404	56.302	36.312
45	485	CE	LYS	791	-3.638	57.635	31.901
	486	NZ	LYS	791	-4.178	58.949	31.508
	487	N	ASN	792	0.120	54.141	36.027
50	488	CA	ASN	792	-0.240	53.788	37.383
	489	CB	ASN	792	-1.030	52.487	37.415
	490	CG	ASN	792	-2.422	52.652	36.853
	491	OD1	ASN	792	-3.101	51.672	36.552
55	492	ND2	ASN	792	-2.974	53.949	36.710
	493	C	ASN	792	1.095	53.627	38.071

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
494	O	ASN	792	1.180	53.287	39.244
495	N	LEU	793	2.153	53.875	37.312
496	CA	LEU	793	3.485	53.780	37.860
497	CB	LEU	793	4.519	53.587	36.745
498	CG	LEU	793	4.503	52.206	36.089
499	CD1	LEU	793	5.496	52.158	34.949
500	CD2	LEU	793	4.844	51.160	37.133
501	C	LEU	793	3.743	55.069	38.610
502	O	LEU	793	3.089	56.089	38.368
503	N	PRO	794	4.688	55.017	39.536
504	CA	PRO	794	5.007	56.194	40.313
505	CB	PRO	794	6.158	55.901	41.257
506	C	PRO	794	5.387	57.333	39.374
507	O	PRO	794	6.407	57.247	38.695
508	CG	PRO	794	6.975	54.906	40.416
509	CD	PRO	794	5.907	54.014	39.774
510	N	LEU	795	4.575	58.390	39.335
511	CA	LEU	795	4.854	59.521	38.455
512	CB	LEU	795	4.144	60.790	38.942
513	CG	LEU	795	4.450	62.072	38.145
514	CD1	LEU	795	3.440	63.137	38.497
515	CD2	LEU	795	5.857	62.592	38.441
516	C	LEU	795	6.348	59.801	38.317
517	O	LEU	795	6.769	60.390	37.324
518	N	GLU	796	7.144	59.401	39.303
519	CA	GLU	796	8.594	59.611	39.238
520	CB	GLU	796	9.257	59.516	40.604
521	C	GLU	796	9.251	58.572	38.367
522	O	GLU	796	10.315	58.816	37.809
523	CG	GLU	796	10.791	59.813	40.678
524	CD	GLU	796	11.462	59.829	42.054
525	OE1	GLU	796	10.836	59.739	43.101
526	OE2	GLU	796	12.818	59.952	42.001
527	N	ASP	797	8.635	57.391	38.316
528	CA	ASP	797	9.107	56.271	37.501
529	CB	ASP	797	8.383	54.968	37.863

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	530	CG	ASP	797	8.665	54.507	39.275
	531	OD1	ASP	797	9.833	54.606	39.707
10	532	OD2	ASP	797	7.718	54.035	39.945
	533	C	ASP	797	8.751	56.630	36.074
	534	O	ASP	797	9.563	56.517	35.157
	535	N	GLN	798	7.505	57.058	35.905
15	536	CA	GLN	798	7.024	57.464	34.610
	537	CB	GLN	798	5.731	58.245	34.769
	538	CG	GLN	798	4.565	57.314	34.706
20	539	CD	GLN	798	3.234	57.989	34.856
	540	OE1	GLN	798	2.991	59.060	34.288
	541	NE2	GLN	798	2.451	57.562	35.945
	542	C	GLN	798	8.087	58.294	33.928
25	543	O	GLN	798	8.230	58.244	32.704
	544	N	ILE	799	8.859	59.014	34.744
	545	CA	ILE	799	9.945	59.891	34.300
30	546	CB	ILE	799	10.055	61.119	35.215
	547	C	ILE	799	11.341	59.269	34.219
	548	O	ILE	799	12.199	59.805	33.514
	549	CG2	ILE	799	11.139	62.134	34.736
35	550	CG1	ILE	799	8.718	61.899	35.423
	551	CD1	ILE	799	8.711	62.930	36.571
	552	N	THR	800	11.614	58.187	34.943
40	553	CA	THR	800	12.959	57.615	34.862
	554	CB	THR	800	13.318	56.724	36.081
	555	OG1	THR	800	12.556	56.983	37.258
	556	CG2	THR	800	14.781	56.946	36.483
45	557	C	THR	800	13.011	56.767	33.604
	558	O	THR	800	14.017	56.733	32.883
	559	N	LEU	801	11.899	56.083	33.354
50	560	CA	LEU	801	11.769	55.242	32.183
	561	CB	LEU	801	10.417	54.506	32.226
	562	CG	LEU	801	10.393	53.076	32.791
	563	CD1	LEU	801	11.605	52.841	33.658
55	564	CD2	LEU	801	9.110	52.836	33.568
	565	C	LEU	801	11.914	56.102	30.918

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
566	O	LEU	801	12.701	55.763	30.037
567	N	ILE	802	11.208	57.228	30.833
568	CA	ILE	802	11.323	58.067	29.641
569	CB	ILE	802	10.281	59.172	29.675
570	C	ILE	802	12.703	58.668	29.396
571	O	ILE	802	13.146	58.779	28.251
572	CG2	ILE	802	10.291	60.052	28.387
573	CG1	ILE	802	8.817	58.681	29.916
574	CD1	ILE	802	7.790	59.774	30.275
575	N	GLN	803	13.385	59.047	30.473
576	CA	GLN	803	14.713	59.645	30.380
577	CB	GLN	803	15.049	60.371	31.662
578	CG	GLN	803	14.189	61.560	31.931
579	CD	GLN	803	14.417	62.099	33.320
580	OE1	GLN	803	14.007	63.217	33.631
581	NE2	GLN	803	15.012	61.291	34.324
582	C	GLN	803	15.778	58.609	30.157
583	O	GLN	803	16.896	58.911	29.733
584	N	TYR	804	15.455	57.378	30.473
585	CA	TYR	804	16.440	56.352	30.278
586	CB	TYR	804	16.211	55.236	31.272
587	CG	TYR	804	16.847	55.463	32.612
588	CD1	TYR	804	17.000	56.745	33.149
589	CE1	TYR	804	17.576	56.924	34.403
590	CD2	TYR	804	17.279	54.382	33.352
591	CE2	TYR	804	17.842	54.543	34.590
592	CZ	TYR	804	17.993	55.802	35.112
593	OH	TYR	804	18.526	55.969	36.371
594	C	TYR	804	16.322	55.808	28.878
595	O	TYR	804	17.320	55.564	28.207
596	N	SER	805	15.085	55.671	28.427
597	CA	SER	805	14.819	55.079	27.130
598	CB	SER	805	13.733	54.018	27.296
599	OG	SER	805	12.460	54.582	27.593
600	C	SER	805	14.439	55.972	25.956
601	O	SER	805	14.044	55.457	24.912

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	602	N	TRP	806	14.563	57.284	26.086
	603	CA	TRP	806	14.169	58.124	24.968
10	604	CB	TRP	806	14.217	59.619	25.378
	605	CG	TRP	806	15.580	60.225	25.512
	606	CD2	TRP	806	16.283	60.932	24.488
	607	CE2	TRP	806	17.566	61.242	24.996
15	608	CE3	TRP	806	15.941	61.369	23.202
	609	CD1	TRP	806	16.442	60.117	26.570
	610	NE1	TRP	806	17.644	60.720	26.265
20	611 1	CZ2	TRP	806	18.530	61.913	24.243
	612	CZ3	TRP	806	16.888	62.037	22.454
	613	CH2	TRP	806	18.166	62.320	22.983
	614	C	TRP	806	14.938	57.847	23.648
25	615	O	TRP	806	14.360	57.934	22.560
	616	N	MET	807	16.213	57.477	23.720
	617	CA	MET	807	16.948	57.218	22.482
30	618	CB	MET	807	18.447	57.385	22.706
	619	CG	MET	807	19.273	57.315	21.430
	620	SD	MET	807	19.210	58.799	20.405
	621	CE	MET	807	20.498	59.740	21.131
35	622	C	MET	807	16.648	55.813	21.956
	623	O	MET	807	16.531	55.594	20.746
	624	N	CYS	808	16.532	54.861	22.870
40	625	CA	CYS	808	16.219	53.498	22.483
	626	CB	CYS	808	15.888	52.536	23.651
	627	C	CYS	808	14.977	53.612	21.599
	628	O	CYS	808	14.928	53.066	20.498
45	629	SG	CYS	808	16.909	52.717	25.155
	630	N	LEU	809	13.995	54.372	22.084
	631	CA	LEU	809	12.724	54.608	21.393
50	632	CB	LEU	809	11.788	55.409	22.288
	633	CG	LEU	809	11.389	54.821	23.629
	634	CD1	LEU	809	10.765	55.921	24.466
	635	CD2	LEU	809	10.440	53.655	23.429
55	636	C	LEU	809	12.844	55.364	20.070
	637	O	LEU	809	12.258	54.966	19.068

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
638	N	SER	810	13.564	56.481	20.102
639	CA	SER	810	13.757	57.322	18.930
640	CB	SER	810	14.560	58.614	19.213
641	C	SER	810	14.486	56.544	17.826
642	O	SER	810	14.054	56.542	16.672
643	OG	SER	810	13.900	59.523	20.087
644	N	SER	811	15.570	55.852	18.181
645	CA	SER	811	16.311	55.075	17.189
646	CB	SER	811	17.662	54.604	17.786
647	C	SER	811	15.555	53.823	16.742
648	O	SER	811	15.607	53.465	15.569
649	OG	SER	811	18.474	53.915	16.843
650	N	PHE	812	14.853	53.150	17.644
651	CA	PHE	812	14.108	51.963	17.235
652	CB	PHE	812	13.521	51.232	18.454
653	CG	PHE	812	12.934	49.891	18.122
654	CD1	PHE	812	13.739	48.872	17.624
655	CD2	PHE	812	11.569	49.676	18.214
656	CE1	PHE	812	13.195	47.657	17.222
657	CE2	PHE	812	11.011	48.450	17.812
658	CZ	PHE	812	11.827	47.446	17.310
659	C	PHE	812	12.985	52.339	16.243
660	O	PHE	812	12.573	51.528	15.408
661	N	ALA	813	12.495	53.570	16.323
662	CA	ALA	813	11.446	54.012	15.416
663	CB	ALA	813	10.748	55.228	15.974
664	C	ALA	813	12.025	54.327	14.038
665	O	ALA	813	11.487	53.875	13.025
666	N	LEU	814	13.104	55.109	13.987
667	CA	LEU	814	13.724	55.420	12.700
668	CB	LEU	814	14.965	56.293	12.899
669	CG	LEU	814	15.989	56.573	11.792
670	CD1	LEU	814	15.697	57.812	10.905
671	CD2	LEU	814	17.278	56.803	12.556
672	C	LEU	814	14.079	54.080	12.050
673	O	LEU	814	13.740	53.851	10.888

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	674	N	SER	815	14.728	53.177	12.790
	675	CA	SER	815	15.034	51.888	12.204
10	676	C	SER	815	13.831	51.476	11.361
	677	O	SER	815	13.916	51.310	10.148
	678	CB	SER	815	15.238	50.928	13.368
	679	OG	SER	815	15.627	49.668	12.894
15	680	N	TRP	816	12.685	51.361	12.019
	681	CA	TRP	816	11.434	50.978	11.379
	682	CB	TRP	816	10.315	51.055	12.403
20	683	CG	TRP	816	9.047	50.515	11.895
	684	CD2	TRP	816	8.731	49.134	11.739
	685	CE2	TRP	816	7.411	49.065	11.243
	686	CE3	TRP	816	9.462	47.951	11.926
25	687	CD1	TRP	816	7.930	51.215	11.522
	688	NE1	TRP	816	6.939	50.341	11.139
	689	CZ2	TRP	816	6.775	47.845	10.988
30	690	CZ3	TRP	816	8.835	46.731	11.667
	691	CH2	TRP	816	7.504	46.690	11.180
	692	C	TRP	816	11.010	51.780	10.145
	693	O	TRP	816	10.683	51.213	9.110
35	694	N	ARG	817	10.969	53.099	10.266
	695	CA	ARG	817	10.557	53.921	9.143
	696	CB	ARG	817	10.573	55.403	9.531
40	697	CG	ARG	817	9.526	55.805	10.563
	698	CD	ARG	817	9.295	57.307	10.536
	699	NE	ARG	817	10.508	58.059	10.853
	700	CZ	ARG	817	11.111	58.023	12.035
45	701	NH1	ARG	817	10.639	57.318	13.120
	702	NH2	ARG	817	12.266	58.742	12.185
	703	C	ARG	817	11.509	53.676	7.978
50	704	O	ARG	817	11.117	53.731	6.809
	705	N	SER	818	12.756	53.381	8.314
	706	CA	SER	818	13.786	53.127	7.321
	707	CB	SER	818	15.145	53.168	7.986
55	708	OG	SER	818	15.502	54.445	8.498
	709	C	SER	818	13.614	51.810	6.609

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
5	710	O	SER	818	13.688	51.727	5.385
	711	N	TYR	819	13.409	50.767	7.383
	712	CA	TYR	819	13.229	49.477	6.787
10	713	CB	TYR	819	13.071	48.486	7.923
	714	CG	TYR	819	12.184	47.309	7.698
	715	CD1	TYR	819	12.514	46.302	6.796
15	716	CE1	TYR	819	11.782	45.115	6.751
	717	CD2	TYR	819	11.087	47.115	8.532
	718	CE2	TYR	819	10.353	45.948	8.494
	719	CZ	TYR	819	10.704	44.948	7.616
20	720	OH	TYR	819	9.962	43.786	7.582
	721	C	TYR	819	12.008	49.556	5.874
	722	O	TYR	819	12.083	49.263	4.685
25	723	N	LYS	820	10.905	50.032	6.412
	724	CA	LYS	820	9.666	50.118	5.652
	725	CB	LYS	820	8.555	50.467	6.636
	726	CG	LYS	820	7.247	50.738	5.915
30	727	CD	LYS	820	6.567	49.442	5.644
	728	C	LYS	820	9.616	51.061	4.440
	729	O	LYS	820	8.699	50.967	3.621
35	730	CE	LYS	820	5.244	49.709	4.914
	731	NZ	LYS	820	4.568	48.428	4.643
	732	N	HIS	821	10.606	51.940	4.292
	733	CA	HIS	821	10.583	52.921	3.208
40	734	CB	HIS	821	10.437	54.309	3.843
	735	C	HIS	821	11.787	52.899	2.268
	736	O	HIS	821	12.029	53.863	1.545
45	737	CG	HIS	821	9.186	55.009	3.400
	738	ND1	HIS	821	8.237	54.502	2.516
	739	CD2	HIS	821	8.840	56.279	3.843
	740	CE1	HIS	821	7.366	55.529	2.498
50	741	NE2	HIS	821	7.651	56.623	3.254
	742	N	THR	822	12.538	51.803	2.266
	743	CA	THR	822	13.716	51.707	1.413
55	744	CB	THR	822	14.564	52.989	1.506
	745	C	THR	822	14.547	50.512	1.846

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	746	O	THR	822	15.775	50.564	1.832
	747	OG1	THR	822	13.817	54.114	1.061
10	748	CG2	THR	822	15.853	53.021	0.656
	749	N	ASN	823	13.871	49.445	2.243
	750	CA	ASN	823	14.534	48.220	2.692
	751	CB	ASN	823	15.012	47.386	1.485
15	752	C	ASN	823	15.748	48.439	3.611
	753	O	ASN	823	16.647	47.601	3.634
	754	CG	ASN	823	13.948	46.974	0.462
20	755	OD1	ASN	823	13.800	47.565	-0.598
	756	ND2	ASN	823	13.160	45.972	0.742
	757	N	SER	824	15.808	49.544	4.349
	758	CA	SER	824	16.954	49.752	5.244
25	759	CB	SER	824	17.191	48.480	6.076
	760	C	SER	824	18.265	50.165	4.543
	761	O	SER	824	19.360	49.892	5.060
30	762	OG	SER	824	17.680	47.386	5.293
	763	N	GLN	825	18.143	50.818	3.385
	764	CA	GLN	825	19.282	51.297	2.587
	765	CB	GLN	825	18.906	51.322	1.097
35	766	C	GLN	825	19.584	52.736	3.015
	767	O	GLN	825	20.737	53.162	3.140
	768	CG	GLN	825	20.033	51.767	0.108
40	769	CD	GLN	825	19.715	51.875	-1.389
	770	OE1	GLN	825	20.556	52.257	-2.187
	771	NE2	GLN	825	18.517	51.579	-1.825
	772	N	PHE	826	18.496	53.472	3.223
45	773	CA	PHE	826	18.522	54.867	3.621
	774	CB	PHE	826	17.631	55.670	2.652
	775	C	PHE	826	18.014	54.998	5.074
50	776	O	PHE	826	17.453	54.048	5.623
	777	CG	PHE	826	18.000	55.595	1.162
	778	CD1	PHE	826	17.467	54.574	0.368
	779	CD2	PHE	826	18.910	56.497	0.605
55	780	CE1	PHE	826	17.853	54.445	-0.962
	781	CE2	PHE	826	19.288	56.374	-0.729

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
782	CZ	PHE	826	18.762	55.347	-1.511
783	N	LEU	827	18.251	56.154	5.696
784	CA	LEU	827	17.788	56.453	7.058
785	CB	LEU	827	18.886	57.119	7.902
786	CG	LEU	827	19.920	56.225	8.582
787	CD1	LEU	827	20.807	57.060	9.505
788	CD2	LEU	827	19.202	55.145	9.369
789	C	LEU	827	16.669	57.452	6.843
790	O	LEU	827	16.913	58.551	6.372
791	N	TYR	828	15.441	57.090	7.191
792	CA	TYR	828	14.331	58.004	6.948
793	CB	TYR	828	13.148	57.169	6.351
794	C	TYR	828	13.884	58.813	8.148
795	O	TYR	828	12.825	58.556	8.710
796	CG	TYR	828	13.150	57.149	4.832
797	CD1	TYR	828	14.257	56.721	4.017
798	CD2	TYR	828	11.970	57.613	4.164
799	CE1 1	TYR	828	14.156	56.768	2.578
800	CE2	TYR	828	11.858	57.630	2.734
801	CZ	TYR	828	12.951	57.195	1.913
802	OH	TYR	828	12.850	57.211	0.539
803	N	PHE	829	14.660	59.812	8.535
804	CA	PHE	829	14.262	60.597	9.684
805	CB	PHE	829	15.320	61.671	9.972
806	CG	PHE	829	16.625	61.104	10.525
807	CD1	PHE	829	17.590	60.544	9.688
808	CD2	PHE	829	16.893	61.149	11.891
809	CE1	PHE	829	18.803	60.037	10.205
810	CE2	PHE	829	18.093	60.642	12.411
811	CZ	PHE	829	19.049	60.094	11.567
812	C	PHE	829	12.815	61.141	9.542
813	O	PHE	829	12.088	61.226	10.530
814	N	ALA	830	12.389	61.465	8.323
815	CA	ALA	830	11.012	61.912	8.054
816	CB	ALA	830	10.922	63.421	8.091
817	C	ALA	830	10.751	61.380	6.641

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	818	O	ALA	830	11.690	61.306	5.852
	819	N	PRO	831	9.507	60.970	6.295
10	820	CD	PRO	831	8.262	60.670	7.030
	821	CA	PRO	831	9.417	60.478	4.911
	822	CB	PRO	831	7.961	60.011	4.804
	823	CG	PRO	831	7.665	59.539	6.198
15	824	C	PRO	831	9.790	61.542	3.867
	825	O	PRO	831	9.926	61.245	2.674
	826	N	ASP	832	9.977	62.772	4.352
20	827	CA	ASP	832	10.339	63.935	3.539
	828	CB	ASP	832	9.543	65.143	3.974
	829	CG	ASP	832	10.046	65.683	5.300
	830	OD1	ASP	832	10.054	64.891	6.255
25	831	OD2	ASP	832	10.454	66.863	5.392
	832	C	ASP	832	11.798	64.340	3.753
	833	O	ASP	832	12.284	65.254	3.090
30	834	N	LEU	833	12.472	63.722	4.713
	835	CA	LEU	833	13.861	64.082	4.992
	836	CB	LEU	833	13.930	64.909	6.282
	837	CG	LEU	833	15.281	65.514	6.662
35	838	CD1	LEU	833	16.340	64.441	6.845
	839	CD2	LEU	833	15.696	66.464	5.573
	840	C	LEU	833	14.716	62.823	5.121
40	841	O	LEU	833	14.824	62.254	6.207
	842	N	VAL	834	15.334	62.407	4.019
	843	CA	VAL	834	16.158	61.190	3.977
	844	CB	VAL	834	15.808	60.368	2.693
45	845	C	VAL	834	17.674	61.416	3.967
	846	O	VAL	834	18.170	62.415	3.448
	847	CG1	VAL	834	16.396	60.934	1.376
50	848	CG2	VAL	834	14.282	60.184	2.512
	849	N	PHE	835	18.416	60.488	4.560
	850	CA	PHE	835	19.854	60.616	4.494
	851	CB	PHE	835	20.630	60.228	5.745
55	852	C	PHE	835	20.280	59.596	3.485
	853	O	PHE	835	20.286	58.387	3.725

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
854	CG	PHE	835	20.548	61.224	6.842
855	CD1	PHE	835	19.878	62.496	6.797
856	CD2	PHE	835	21.319	60.857	7.977
857	CE1	PHE	835	20.101	63.432	7.850
858	CE2	PHE	835	21.570	61.796	9.005
859	CZ	PHE	835	21.027	63.115	8.896
860	N	ASN	836	20.603	60.152	2.328
861	CA	ASN	836	21.032	59.451	1.146
862	CB	ASN	836	20.450	60.127	-0.060
863	CG	ASN	836	20.793	61.596	-0.078
864	OD1	ASN	836	21.630	62.058	0.693
865	ND2	ASN	836	20.115	62.368	-1.049
866	C	ASN	836	22.534	59.501	0.992
867	O	ASN	836	23.249	60.240	1.687
868	N	GLU	837	22.949	58.760	-0.032
869	CA	GLU	837	24.329	58.541	-0.415
870	CB	GLU	837	24.396	57.808	-1.742
871	CG	GLU	837	25.840	57.675	-2.174
872	CD	GLU	837	26.031	57.213	-3.602
873	OE1	GLU	837	26.427	58.052	-4.450
874	OE2	GLU	837	25.794	56.012	-3.869
875	C	GLU	837	25.227	59.722	-0.535
876	O	GLU	837	26.416	59.668	-0.228
877	N	GLU	838	24.647	60.782	-1.040
878	CA	GLU	838	25.378	61.978	-1.248
879	CB	GLU	838	24.642	62.790	-2.263
880	CG	GLU	838	25.038	62.639	-3.742
881	CD	GLU	838	26.168	61.663	-4.134
882	OE1	GLU	838	27.334	61.821	-3.776
883	C	GLU	838	25.407	62.686	0.081
884	O	GLU	838	26.369	63.362	0.419
885	OE2	GLU	838	25.730	60.547	-4.780
886	N	LYS	839	24.345	62.521	0.845
887	CA	LYS	839	24.288	63.151	2.151
888	CB	LYS	839	22.863	63.198	2.639
889	CG	LYS	839	22.311	64.577	2.459

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
5	890	CD	LYS	839	20.763	64.663	2.497
	891	C	LYS	839	25.096	62.361	3.137
10	892	O	LYS	839	25.659	62.856	4.103
	893	CE	LYS	839	20.171	65.129	3.825
	894	NZ	LYS	839	18.664	65.315	3.753
	895	N	MET	840	25.122	61.087	2.878
15	896	CA	MET	840	25.789	60.159	3.731
	897	CB	MET	840	25.603	58.818	3.159
	898	CG	MET	840	25.733	57.886	4.225
20	899	SD	MET	840	25.047	58.641	5.697
	900	CE	MET	840	24.686	57.251	6.529
	901	C	MET	840	27.226	60.385	3.766
	902	O	MET	840	28.007	59.936	4.606
25	903	N	HIS	841	27.573	61.081	2.751
	904	CA	HIS	841	28.906	61.294	2.575
	905	CB	HIS	841	29.072	61.097	1.163
30	906	C	HIS	841	29.329	62.646	3.089
	907	O	HIS	841	30.409	63.072	2.743
	908	CG	HIS	841	30.015	59.972	0.852
	909	ND1	HIS	841	30.678	59.182	1.788
35	910	CD2	HIS	841	30.332	59.596	-0.446
	911	CE1	HIS	841	31.356	58.365	0.960
	912	NE2	HIS	841	31.210	58.546	-0.381
40	913	N	GLN	842	28.541	63.372	3.892
	914	CA	GLN	842	29.156	64.615	4.349
	915	CB	GLN	842	28.132	65.700	4.833
	916	C	GLN	842	30.070	64.165	5.438
45	917	O	GLN	842	30.086	62.991	5.841
	918	CG	GLN	842	27.078	65.394	5.944
	919	CD	GLN	842	27.589	65.356	7.401
50	920	OE1	GLN	842	28.755	65.223	7.682
	921	NE2	GLN	842	26.648	65.484	8.434
	922	N	SER	843	30.830	65.108	5.957
	923	CA	SER	843	31.759	64.768	7.003
55	924	CB	SER	843	32.336	66.099	7.608
	925	C	SER	843	31.391	63.778	8.034

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
926	O	SER	843	31.420	62.553	7.872
927	OG	SER	843	33.011	66.917	6.653
928	N	ALA	844	30.999	64.345	9.132
929	CA	ALA	844	30.810	63.473	10.210
930	CB	ALA	844	31.009	64.296	11.460
931	C	ALA	844	29.573	62.635	10.269
932	O	ALA	844	29.221	62.183	11.333
933	N	MET	845	28.968	62.331	9.135
934	CA	MET	845	27.710	61.611	9.171
935	CB	MET	845	26.946	61.885	7.902
936	CG	MET	845	25.462	61.900	8.075
937	SD	MET	845	24.889	63.585	7.922
938	CE	MET	845	24.327	63.891	9.531
939	C	MET	845	27.725	60.135	9.325
940	O	MET	845	27.067	59.529	10.174
941	N	TYR	846	28.451	59.556	8.404
942	CA	TYR	846	28.495	58.155	8.351
943	CB	TYR	846	29.415	57.741	7.245
944	CG	TYR	846	29.192	56.313	7.082
945	CD1	TYR	846	28.044	55.867	6.448
946	CE1	TYR	846	27.676	54.551	6.503
947	CD2	TYR	846	29.983	55.399	7.763
948	CE2	TYR	846	29.627	54.082	7.832
949	CZ	TYR	846	28.470	53.663	7.203
950	OH	TYR	846	28.093	52.340	7.273
951	C	TYR	846	28.882	57.431	9.614
952	O	TYR	846	28.392	56.346	9.902
953	N	GLU	847	29.778	58.022	10.375
954	CA	GLU	847	30.229	57.375	11.588
955	CB	GLU	847	31.460	58.107	12.190
956	C	GLU	847	29.169	57.332	12.645
957	O	GLU	847	29.200	56.488	13.527
958	CG	GLU	847	32.714	58.107	11.274
959	CD	GLU	847	32.724	59.178	10.124
960	OE1	GLU	847	31.953	60.136	10.244
961	OE2	GLU	847	33.520	58.935	9.212

TABLE 11 (continued)

	THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP						
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	962	N	LEU	848	28.273	58.308	12.559
	963	CA	LEU	848	27.154	58.520	13.459
10	964	CB	LEU	848	26.290	59.841	13.644
	965	C	LEU	848	25.982	57.658	12.978
	966	O	LEU	848	25.422	56.844	13.718
	967	CG	LEU	848	26.887	61.083	14.323
15	968	CD1	LEU	848	27.925	61.493	13.330
	969	CD2	LEU	848	26.178	62.437	14.532
	970	N	CYS	849	25.650	57.839	11.701
20	971	CA	CYS	849	24.532	57.155	11.019
	972	CB	CYS	849	24.405	57.671	9.579
	973	SG	CYS	849	23.678	59.351	9.531
	974	C	CYS	849	24.543	55.623	10.958
25	975	O	CYS	849	23.506	54.988	10.769
	976	N	GLN	850	25.715	55.048	11.133
	977	CA	GLN	850	25.944	53.608	11.062
30	978	CB	GLN	850	27.406	53.378	11.325
	979	CG	GLN	850	27.924	51.916	11.314
	980	C	GLN	850	25.184	52.763	12.043
	981	O	GLN	850	24.733	51.634	11.793
35	982	CD	GLN	850	27.809	51.215	12.681
	983	OE1	GLN	850	27.149	50.200	12.827
	984	NE2	GLN	850	28.565	51.802	13.727
40	985	N	GLY	851	25.145	53.330	13.217
	986	CA	GLY	851	24.522	52.700	14.298
	987	C	GLY	851	23.106	52.528	14.083
	988	O	GLY	851	22.547	51.454	14.255
45	989	N	MET	852	22.519	53.591	13.607
	990	CA	MET	852	21.140	53.494	13.346
	991	CB	MET	852	20.608	54.871	13.110
50	992	CG	MET	852	20.424	55.544	14.421
	993	SD	MET	852	21.486	56.946	14.587
	994	CE	MET	852	20.673	58.004	13.550
	995	C	MET	852	20.810	52.578	12.197
55	996	O	MET	852	19.837	51.835	12.279
	997	N	HIS	853	21.612	52.609	11.129

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
998	CA	HIS	853	21.304	51.767	9.970
999	CB	HIS	853	22.420	52.169	8.960
1000	C	HIS	853	21.379	50.345	10.421
1001	O	HIS	853	20.659	49.469	9.951
1002	CG	HIS	853	22.400	51.593	7.579
1003	ND1	HIS	853	23.387	50.809	7.081
1004	CD2	HIS	853	21.537	51.981	6.514
1005	CE1	HIS	853	23.138	50.710	5.752
1006	NE2	HIS	853	21.998	51.423	5.314
1007	N	GLN	854	22.262	50.110	11.355
1008	CA	GLN	854	22.339	48.801	11.876
1009	CB	GLN	854	23.440	48.628	12.964
1010	C	GLN	854	20.984	48.364	12.473
1011	O	GLN	854	20.608	47.196	12.391
1012	CG	GLN	854	24.048	47.211	13.119
1013	CD	GLN	854	23.110	46.185	13.774
1014	OE1	GLN	854	22.675	45.231	13.152
1015	NE2	GLN	854	22.838	46.395	15.146
1016	N	ILE	855	20.241	49.258	13.103
1017	CA	ILE	855	19.007	48.728	13.636
1018	CB	ILE	855	18.540	49.626	14.847
1019	C	ILE	855	18.008	48.491	12.500
1020	O	ILE	855	17.340	47.453	12.470
1021	CG2	ILE	855	18.443	51.150	14.670
1022	CG1	ILE	855	17.328	49.137	15.655
1023	CD1	ILE	855	17.540	47.718	16.167
1024	N	SER	856	17.957	49.403	11.534
1025	CA	SER	856	17.062	49.251	10.377
1026	CB	SER	856	17.225	50.415	9.416
1027	OG	SER	856	16.618	50.174	8.183
1028	C	SER	856	17.331	47.979	9.573
1029	O	SER	856	16.412	47.323	9.066
1030	N	LEU	857	18.611	47.666	9.421
1031	CA	LEU	857	19.038	46.485	8.683
1032	CB	LEU	857	20.575	46.447	8.642
1033	C	LEU	857	18.502	45.237	9.374

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1034	O	LEU	857	17.965	44.322	8.748
	1035	CG	LEU	857	21.320	47.661	8.023
10	1036	CD1	LEU	857	22.829	47.385	7.974
	1037	CD2	LEU	857	20.812	48.015	6.616
	1038	N	GLN	858	18.650	45.240	10.691
15	1039	CA	GLN	858	18.238	44.144	11.542
	1040	CB	GLN	858	18.684	44.468	12.954
	1041	CG	GLN	858	19.288	43.311	13.700
20	1042	CD	GLN	858	20.205	42.435	12.870
	1043	OE1	GLN	858	20.787	42.893	11.862
	1044	C	GLN	858	16.746	43.849	11.479
25	1045	O	GLN	858	16.340	42.686	11.548
	1046	NE2	GLN	858	20.290	41.153	13.122
	1047	N	PHE	859	15.939	44.899	11.363
30	1048	CA	PHE	859	14.487	44.761	11.249
	1049	CB	PHE	859	13.657	46.030	11.128
	1050	C	PHE	859	14.240	44.094	9.903
35	1051	O	PHE	859	13.519	43.102	9.792
	1052	CG	PHE	859	13.725	46.803	12.385
	1053	CD1	PHE	859	14.553	46.478	13.511
40	1054	CD2	PHE	859	12.875	47.932	12.422
	1055	CE1	PHE	859	14.586	47.350	14.620
	1056	CE2	PHE	859	12.808	48.720	13.599
45	1057	CZ	PHE	859	13.718	48.480	14.649
	1058	N	VAL	860	14.871	44.645	8.879
	1059	CA	VAL	860	14.758	44.135	7.528
50	1060	CB	VAL	860	15.677	44.943	6.610
	1061	C	VAL	860	15.115	42.651	7.454
	1062	O	VAL	860	14.315	41.819	7.012
55	1063	CG1	VAL	860	15.273	46.430	6.469
	1064	CG2	VAL	860	15.831	44.420	5.154
	1065	N	ARG	861	16.326	42.334	7.893
60	1066	CA	ARG	861	16.825	40.972	7.892
	1067	CB	ARG	861	18.162	40.913	8.593
	1068	CG	ARG	861	18.870	39.604	8.405
65	1069	CD	ARG	861	19.848	39.390	9.514

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
1070	NE	ARG	861	19.228	38.616	10.571
1071	CZ	ARG	861	19.711	38.535	11.801
1072	NH1	ARG	861	20.935	39.043	12.107
1073	NH2	ARG	861	19.004	37.885	12.767
1074	C	ARG	861	15.898	40.026	8.614
1075	O	ARG	861	15.741	38.865	8.228
1076	N	LEU	862	15.297	40.508	9.689
1077	CA	LEU	862	14.413	39.666	10.468
1078	CB	LEU	862	14.535	40.041	11.944
1079	CG	LEU	862	15.646	39.262	12.636
1080	CD1	LEU	862	15.630	39.590	14.115
1081	CD2	LEU	862	15.417	37.773	12.426
1082	C	LEU	862	12.952	39.682	10.028
1083	O	LEU	862	12.119	38.979	10.620
1084	N	GLN	863	12.680	40.448	8.965
1085	CA	GLN	863	11.340	40.653	8.392
1086	CB	GLN	863	10.916	39.504	7.457
1087	CG	GLN	863	11.428	39.629	5.993
1088	CD	GLN	863	10.976	40.915	5.273
1089	OE1	GLN	863	11.805	41.700	4.789
1090	NE2	GLN	863	9.586	41.107	5.109
1091	C	GLN	863	10.351	40.827	9.514
1092	O	GLN	863	9.407	40.053	9.670
1093	N	LEU	864	10.596	41.870	10.296
1094	CA	LEU	864	9.779	42.199	11.447
1095	CB	LEU	864	10.528	43.160	12.410
1096	C	LEU	864	8.415	42.778	11.107
1097	O	LEU	864	8.271	43.751	10.368
1098	CG	LEU	864	11.894	42.701	12.985
1099	CD1	LEU	864	12.416	43.734	13.994
1100	CD2	LEU	864	11.824	41.317	13.651
1101	N	THR	865	7.429	42.112	11.694
1102	CA	THR	865	5.996	42.362	11.621
1103	CB	THR	865	5.338	41.183	12.351
1104	C	THR	865	5.650	43.704	12.299
1105	O	THR	865	6.383	44.157	13.177

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1106	OG1	THR	865	5.645	39.958	11.697
	1107	CG2	THR	865	3.796	41.202	12.431
10	1108	N	PHE	866	4.549	44.344	11.902
	1109	CA	PHE	866	4.179	45.602	12.542
	1110	CB	PHE	866	2.971	46.256	11.885
	1111 1	CG	PHE	866	2.764	47.665	12.387
15	1112	CD1	PHE	866	3.849	48.527	12.499
	1113	CE1	PHE	866	3.698	49.840	12.880
	1114	CD2	PHE	866	1.491	48.163	12.686
20	1115	CE2	PHE	866	1.325	49.499	13.076
	1116	CZ	PHE	866	2.443	50.328	13.161
	1117	C	PHE	866	3.810	45.338	13.983
	1118	O	PHE	866	4.164	46.095	14.882
25	1119	N	GLU	867	3.068	44.261	14.198
	1120	CA	GLU	867	2.654	43.934	15.538
	1121	CB	GLU	867	1.665	42.778	15.514
30	1122	CG	GLU	867	0.327	43.271	15.008
	1123	CD	GLU	867	-0.811	42.319	15.281
	1124	OE1	GLU	867	-0.557	41.199	15.789
	1125	OE2	GLU	867	-1.968	42.697	14.982
35	1126	C	GLU	867	3.868	43.646	16.384
	1127	O	GLU	867	4.059	44.288	17.417
	1128	N	GLU	868	4.698	42.705	15.947
40	1129	CA	GLU	868	5.907	42.402	16.692
	1130	CB	GLU	868	6.830	41.522	15.870
	1131	CG	GLU	868	6.445	40.076	15.819
	1132	CD	GLU	868	7.082	39.394	14.633
45	1133	OE1	GLU	868	7.563	40.120	13.738
	1134	OE2	GLU	868	7.098	38.145	14.578
	1135	C	GLU	868	6.639	43.703	17.021
50	1136	O	GLU	868	7.153	43.870	18.127
	1137	N	TYR	869	6.682	44.620	16.057
	1138	CA	TYR	869	7.362	45.912	16.220
	1139	CB	TYR	869	7.334	46.717	14.917
55	1140	CG	TYR	869	7.566	48.214	15.110
	1141	CD1	TYR	869	8.841	48.707	15.377

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
1142	CE1	TYR	869	9.078	50.090	15.512
1143	CD2	TYR	869	6.518	49.135	14.988
1144	CE2	TYR	869	6.741	50.522	15.121
1145	CZ	TYR	869	8.031	50.995	15.377
1146	OH	TYR	869	8.278	52.347	15.435
1147	C	TYR	869	6.782	46.823	17.285
1148	O	TYR	869	7.505	47.585	17.942
1149	N	THR	870	5.459	46.790	17.394
1150	CA	THR	870	4.757	47.628	18.332
1151	CB	THR	870	3.267	47.598	18.011
1152	C	THR	870	5.034	47.166	19.744
1153	O	THR	870	5.166	47.973	20.677
1154	OG1	THR	870	3.028	48.107	16.705
1155	CG2	THR	870	2.352	48.438	18.927
1156	N	ILE	871	5.140	45.850	19.877
1157	CA	ILE	871	5.423	45.234	21.144
1158	CB	ILE	871	5.154	43.742	21.054
1159	C	ILE	871	6.861	45.490	21.549
1160	O	ILE	871	7.126	45.921	22.670
1161	CG2	ILE	871	6.045	43.029	19.990
1162	CG1	ILE	871	5.301	42.970	22.405
1163	CD1	ILE	871	4.189	43.217	23.446
1164	N	MET	872	7.799	45.254	20.640
1165	CA	MET	872	9.204	45.461	20.964
1166	CB	MET	872	10.079	45.164	19.745
1167	CG	MET	872	10.038	43.703	19.358
1168	SD	MET	872	10.628	43.346	17.700
1169	CE	MET	872	12.453	43.439	17.963
1170	C	MET	872	9.497	46.859	21.456
1171	O	MET	872	10.363	47.055	22.306
1172	N	LYS	873	8.775	47.837	20.936
1173	CA	LYS	873	9.053	49.209	21.332
1174	CB	LYS	873	8.538	50.163	20.271
1175	CG	LYS	873	8.908	51.591	20.516
1176	CD	LYS	873	8.754	52.389	19.236
1177	CE	LYS	873	7.362	52.259	18.639

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1178	NZ	LYS	873	6.239	53.012	19.336
	1179	C	LYS	873	8.491	49.569	22.700
10	1180	O	LYS	873	8.978	50.493	23.351
	1181	N	VAL	874	7.463	48.847	23.128
	1182	CA	VAL	874	6.866	49.089	24.430
	1183	CB	VAL	874	5.492	48.376	24.544
15	1184	C	VAL	874	7.893	48.487	25.380
	1185	O	VAL	874	8.224	49.083	26.404
	1186	CG1	VAL	874	4.419	48.922	23.572
20	1187	CG2	VAL	874	4.821	48.392	25.946
	1188	N	LEU	875	8.428	47.320	25.008
	1189	CA	LEU	875	9.457	46.653	25.807
	1190	CB	LEU	875	9.812	45.282	25.220
25	1191	CG	LEU	875	8.794	44.155	25.429
	1192	CD1	LEU	875	9.347	42.853	24.943
	1193	CD2	LEU	875	8.470	44.024	26.891
30	1194	C	LEU	875	10.730	47.502	25.899
	1195	O	LEU	875	11.542	47.320	26.800
	1196	N	LEU	876	10.913	48.436	24.982
	1197	CA	LEU	876	12.115	49.251	25.029
35	1198	CB	LEU	876	12.420	49.780	23.628
	1199	CG	LEU	876	13.716	49.452	22.883
	1200	CD1	LEU	876	14.049	47.987	22.801
40	1201	CD2	LEU	876	13.505	49.985	21.502
	1202	C	LEU	876	11.992	50.402	26.028
	1203	O	LEU	876	12.992	50.971	26.459
	1204	N	LEU	877	10.764	50.753	26.385
45	1205	CA	LEU	877	10.515	51.824	27.336
	1206	CB	LEU	877	9.045	52.267	27.204
	1207	CG	LEU	877	8.268	53.010	28.298
50	1208	CD1	LEU	877	8.854	54.379	28.492
	1209	CD2	LEU	877	6.797	53.135	27.915
	1210	C	LEU	877	10.809	51.215	28.712
	1211	O	LEU	877	11.403	51.849	29.592
55	1212	N	LEU	878	10.432	49.948	28.853
	1213	CA	LEU	878	10.611	49.201	30.091

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLOGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
1214	CB	LEU	878	9.394	48.292	30.296
1215	CG	LEU	878	8.073	48.871	29.772
1216	CD1	LEU	878	6.945	47.851	29.885
1217	CD2	LEU	878	7.750	50.136	30.547
1218	C	LEU	878	11.887	48.349	30.075
1219	O	LEU	878	11.906	47.272	30.680
1220	N	SER	879	12.949	48.825	29.416
1221	CA	SER	879	14.183	48.040	29.311
1222	CB	SER	879	14.633	47.944	27.855
1223	OG	SER	879	15.010	49.185	27.276
1224	C	SER	879	15.377	48.434	30.177
1225	O	SER	879	16.435	47.801	30.115
1226	N	THR	880	15.241	49.506	30.945
1227	CA	THR	880	16.306	49.863	31.866
1228	CB	THR	880	17.441	50.658	31.193
1229	C	THR	880	15.672	50.612	33.024
1230	O	THR	880	14.854	51.521	32.838
1231	OG1	THR	880	18.052	49.883	30.170
1232	CG2	THR	880	18.611	51.086	32.105
1233	N	ILE	881	16.011	50.141	34.219
1234	CA	ILE	881	15.529	50.691	35.474
1235	CB	ILE	881	14.715	49.639	36.255
1236	C	ILE	881	16.750	51.096	36.301
1237	O	ILE	881	17.875	50.683	36.007
1238	CG2	ILE	881	14.098	50.207	37.571
1239	CG1	ILE	881	13.571	48.961	35.436
1240	CD1	ILE	881	12.952	47.695	36.064
1241	N	PRO	882	16.541	51.911	37.353
1242	CD	PRO	882	15.213	52.253	37.874
1243	CA	PRO	882	17.583	52.405	38.259
1244	CB	PRO	882	16.793	53.230	39.274
1245	CG	PRO	882	15.491	53.531	38.574
1246	C	PRO	882	18.231	51.194	38.909
1247	O	PRO	882	17.620	50.126	38.947
1248	N	LYS	883	19.445	51.340	39.428
1249	CA	LYS	883	20.117	50.199	40.051

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
10	1250	CB	LYS	883	21.558	50.551	40.430
	1251	CG	LYS	883	22.417	49.338	40.803
	1252	CD	LYS	883	23.224	49.590	42.079
	1253	CE	LYS	883	22.299	49.706	43.280
	1254	NZ	LYS	883	22.861	50.379	44.517
	1255	C	LYS	883	19.355	49.753	41.292
15	1256	O	LYS	883	19.617	48.681	41.849
20	1257	N	ASP	884	18.408	50.581	41.721
	1258	CA	ASP	884	17.606	50.272	42.889
	1259	CB	ASP	884	17.762	51.369	43.940
	1260	CG	ASP	884	19.210	51.672	44.247
25	1261	OD1	ASP	884	20.041	50.750	44.122
	1262	OD2	ASP	884	19.512	52.825	44.627
	1263	C	ASP	884	16.138	50.131	42.515
	1264	O	ASP	884	15.251	50.464	43.303
30	1265	N	GLY	885	15.882	49.635	41.309
	1266	CA	GLY	885	14.507	49.480	40.885
	1267	C	GLY	885	13.772	50.793	41.061
	1268	O	GLY	885	14.325	51.788	41.531
35	1269	N	LEU	886	12.497	50.792	40.704
	1270	CA	LEU	886	11.704	52.001	40.798
	1271	CB	LEU	886	10.794	52.067	39.584
	1272	CG	LEU	886	11.543	51.498	38.387
40	1273	CD1	LEU	886	10.575	50.833	37.457
	1274	CD2	LEU	886	12.319	52.589	37.698
	1275	C	LEU	886	10.886	52.021	42.069
	1276	O	LEU	886	11.072	51.198	42.965
45	1277	N	LYS	887	9.972	52.975	42.154
50	1278	CA	LYS	887	9.131	53.063	43.320
	1279	CB	LYS	887	8.698	54.508	43.562
	1280	CG	LYS	887	7.958	54.747	44.880
	1281	CD	LYS	887	7.695	56.233	45.037
55	1282	CE	LYS	887	6.960	56.606	46.316
	1283	NZ	LYS	887	6.728	58.098	46.415
	1284	C	LYS	887	7.910	52.179	43.139
	1285	O	LYS	887	7.102	52.048	44.051

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1286	N	SER	888	7.763	51.569	41.965
	1287	CA	SER	888	6.615	50.688	41.729
10	1288	CB	SER	888	5.567	51.386	40.850
	1289	OG	SER	888	4.960	52.527	41.454
	1290	C	SER	888	7.027	49.362	41.087
15	1291	O	SER	888	6.225	48.699	40.426
	1292	N	GLN	889	8.283	48.978	41.309
	1293	CA	GLN	889	8.846	47.746	40.773
20	1294	CB	GLN	889	10.035	47.304	41.610
	1295	CG	GLN	889	11.343	47.861	41.125
	1296	CD	GLN	889	11.823	47.197	39.842
25	1297	OE1	GLN	889	12.707	47.715	39.166
	1298	NE2	GLN	889	11.345	45.921	39.490
	1299	C	GLN	889	7.904	46.574	40.640
30	1300	O	GLN	889	8.015	45.800	39.698
	1301	N	ALA	890	6.994	46.410	41.583
	1302	CA	ALA	890	6.090	45.281	41.470
35	1303	CB	ALA	890	5.206	45.180	42.714
	1304	C	ALA	890	5.253	45.430	40.199
	1305	O	ALA	890	5.190	44.502	39.394
40	1306	N	ALA	891	4.638	46.605	40.014
	1307	CA	ALA	891	3.819	46.882	38.830
	1308	CB	ALA	891	3.170	48.281	38.928
45	1309	C	ALA	891	4.707	46.811	37.580
	1310	O	ALA	891	4.391	46.110	36.619
	1311	N	PHE	892	5.821	47.543	37.604
50	1312	CA	PHE	892	6.767	47.547	36.502
	1313	CB	PHE	892	8.095	48.151	36.942
	1314	CG	PHE	892	9.110	48.217	35.852
55	1315	CD1	PHE	892	9.105	49.277	34.959
	1316	CD2	PHE	892	10.025	47.184	35.668
	1317	CE1	PHE	892	10.000	49.328	33.900
55	1318	CE2	PHE	892	10.928	47.218	34.606
	1319	CZ	PHE	892	10.912	48.291	33.716
	1320	C	PHE	892	7.045	46.128	36.016
	1321	O	PHE	892	6.798	45.783	34.860

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1322	N	GLU	893	7.578	45.303	36.908
	1323	CA	GLU	893	7.899	43.935	36.543
10	1324	CB	GLU	893	8.440	43.176	37.770
	1325	C	GLU	893	6.684	43.238	35.929
	1326	O	GLU	893	6.831	42.384	35.055
	1327	CG	GLU	893	7.451	42.934	38.958
15	1328	CD	GLU	893	7.989	42.272	40.229
	1329	OE1	GLU	893	7.298	42.072	41.219
	1330	OE2	GLU	893	9.304	41.928	40.153
20	1331	N	GLU	894	5.491	43.637	36.359
	1332	CA	GLU	894	4.232	43.066	35.869
	1333	CB	GLU	894	3.100	43.444	36.828
	1334	CG	GLU	894	2.259	42.274	37.299
25	1335	CD	GLU	894	0.876	42.263	36.679
	1336	OE1	GLU	894	0.116	43.238	36.905
	1337	OE2	GLU	894	0.552	41.278	35.966
30	1338	C	GLU	894	3.879	43.542	34.455
	1339	O	GLU	894	3.375	42.779	33.628
	1340	N	MET	895	4.121	44.821	34.197
	1341	CA	MET	895	3.848	45.387	32.892
35	1342	CB	MET	895	4.040	46.900	32.930
	1343	C	MET	895	4.847	44.714	31.975
	1344	O	MET	895	4.471	43.967	31.082
40	1345	CG	MET	895	3.096	47.676	33.873
	1346	SD	MET	895	3.257	49.445	33.578
	1347	CE	MET	895	2.384	50.038	35.034
	1348	N	ARG	896	6.134	44.938	32.213
45	1349	CA	ARG	896	7.114	44.290	31.373
	1350	CB	ARG	896	8.462	44.273	32.055
	1351	CG	ARG	896	9.570	43.824	31.153
50	1352	CD	ARG	896	10.755	44.671	31.489
	1353	NE	ARG	896	11.915	44.395	30.662
	1354	CZ	ARG	896	12.544	43.231	30.646
	1355	NH1	ARG	896	12.208	42.170	31.438
55	1356	NH2	ARG	896	13.594	43.080	29.790
	1357	C	ARG	896	6.724	42.853	31.006

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1358	O	ARG	896	6.778	42.484	29.843
	1359	N	THR	897	6.321	42.040	31.982
10	1360	CA	THR	897	5.972	40.649	31.675
	1361	CB	THR	897	5.836	39.832	32.966
	1362	C	THR	897	4.713	40.500	30.812
	1363	O	THR	897	4.537	39.495	30.117
15	1364	OG1	THR	897	7.069	39.810	33.673
	1365	CG2	THR	897	5.460	38.344	32.797
	1366	N	ASN	898	3.840	41.500	30.855
20	1367	CA	ASN	898	2.633	41.463	30.048
	1368	CB	ASN	898	1.627	42.534	30.488
	1369	C	ASN	898	3.027	41.690	28.597
	1370	O	ASN	898	2.551	40.981	27.705
25	1371	CG	ASN	898	0.278	42.560	29.761
	1372	OD1	ASN	898	-0.007	41.755	28.887
	1373	ND2	ASN	898	-0.587	43.488	30.072
30	1374	N	TYR	899	3.901	42.668	28.358
	1375	CA	TYR	899	4.357	42.916	26.993
	1376	CB	TYR	899	4.958	44.319	26.837
	1377	CG	TYR	899	3.898	45.370	26.990
35	1378	CD1	TYR	899	2.761	45.351	26.171
	1379	CE1	TYR	899	1.691	46.186	26.418
	1380	CD2	TYR	899	3.939	46.276	28.047
40	1381	CE2	TYR	899	2.873	47.116	28.304
	1382	CZ	TYR	899	1.747	47.061	27.493
	1383	OH	TYR	899	0.646	47.833	27.786
	1384	C	TYR	899	5.342	41.871	26.485
45	1385	O	TYR	899	5.514	41.745	25.278
	1386	N	ILE	900	6.002	41.120	27.362
	1387	CA	ILE	900	6.888	40.094	26.830
50	1388	CB	ILE	900	7.818	39.464	27.891
	1389	CG2	ILE	900	8.529	38.247	27.308
	1390	CG1	ILE	900	8.885	40.475	28.305
	1391	CD1	ILE	900	9.789	39.977	29.395
55	1392	C	ILE	900	5.966	39.022	26.273
	1393	O	ILE	900	6.308	38.318	25.332

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1394	N	LYS	901	4.774	38.920	26.847
	1395	CA	LYS	901	3.820	37.936	26.375
10	1396	CB	LYS	901	2.807	37.615	27.481
	1397	CG	LYS	901	3.401	36.899	28.709
	1398	CD	LYS	901	2.301	36.662	29.743
	1399	CE	LYS	901	2.768	35.909	30.996
15	1400	NZ	LYS	901	1.690	35.710	32.047
	1401	C	LYS	901	3.116	38.438	25.106
	1402	O	LYS	901	2.877	37.670	24.177
20	1403	N	GLU	902	2.798	39.726	25.065
	1404	CA	GLU	902	2.149	40.312	23.902
	1405	CB	GLU	902	2.008	41.822	24.130
	1406	CG	GLU	902	0.593	42.462	24.051
25	1407	CD	GLU	902	-0.577	41.510	23.728
	1408	OE1	GLU	902	-0.991	40.733	24.621
	1409	OE2	GLU	902	-1.096	41.558	22.584
30	1410	C	GLU	902	3.039	40.011	22.669
	1411	O	GLU	902	2.537	39.667	21.596
	1412	N	LEU	903	4.362	40.131	22.845
	1413	CA	LEU	903	5.363	39.873	21.792
35	1414	CB	LEU	903	6.793	40.172	22.297
	1415	CG	LEU	903	7.966	39.883	21.341
	1416	CD1	LEU	903	7.870	40.820	20.160
40	1417	CD2	LEU	903	9.317	40.065	22.031
	1418	C	LEU	903	5.302	38.420	21.334
	1419	O	LEU	903	5.470	38.121	20.154
	1420	N	ARG	904	5.081	37.516	22.276
45	1421	CA	ARG	904	4.987	36.115	21.925
	1422	C	ARG	904	3.726	35.913	21.116
	1423	O	ARG	904	3.677	35.090	20.209
50	1424	CB	ARG	904	4.966	35.268	23.229
	1425	CG	ARG	904	5.012	33.727	23.027
	1426	CD	ARG	904	4.952	32.966	24.363
	1427	NE	ARG	904	5.000	31.497	24.107
55	1428	CZ	ARG	904	4.968	30.552	25.043
	1429	NH1	ARG	904	5.024	29.314	24.667

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
5	1430	NH2	ARG	904	4.882	30.803	26.319
	1431	N	LYS	905	2.694	36.677	21.447
	1432	CA	LYS	905	1.443	36.573	20.714
10	1433	CB	LYS	905	0.381	37.420	21.376
	1434	CG	LYS	905	-0.197	36.796	22.603
	1435	CD	LYS	905	-1.091	37.799	23.250
15	1436	CE	LYS	905	-2.163	37.147	24.059
	1437	NZ	LYS	905	-3.222	38.155	24.471
	1438	C	LYS	905	1.650	37.048	19.291
	1439	O	LYS	905	1.153	36.432	18.342
20	1440	N	MET	906	2.383	38.151	19.153
	1441	CA	MET	906	2.678	38.711	17.851
	1442	CB	MET	906	3.582	39.912	18.000
25	1443	C	MET	906	3.358	37.635	17.025
	1444	O	MET	906	2.876	37.279	15.958
	1445	CG	MET	906	2.996	41.101	18.791
	1446	SD	MET	906	4.072	42.535	18.622
30	1447	CE	MET	906	3.361	43.556	19.919
	1448	N	VAL	907	4.476	37.114	17.539
	1449	CA	VAL	907	5.262	36.053	16.882
35	1450	CB	VAL	907	6.249	35.411	17.901
	1451	C	VAL	907	4.369	34.951	16.314
	1452	O	VAL	907	4.371	34.664	15.112
40	1453	CG1	VAL	907	7.338	36.382	18.418
	1454	CG2	VAL	907	7.019	34.152	17.415
	1455	N	THR	908	3.616	34.336	17.209
	1456	CA	THR	908	2.694	33.268	16.880
45	1457	CB	THR	908	1.867	32.900	18.119
	1458	C	THR	908	1.735	33.600	15.736
	1459	O	THR	908	1.647	32.855	14.760
50	1460	OG1	THR	908	2.713	32.433	19.162
	1461	CG2	THR	908	0.822	31.778	17.937
	1462	N	LYS	909	1.004	34.701	15.878
	1463	CA	LYS	909	0.033	35.157	14.877
55	1464	CB	LYS	909	-0.430	36.583	15.254
	1465	CG	LYS	909	-1.811	37.037	14.735

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TABLE 11 (continued)

	THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP						
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1466	CD	LYS	909	-2.258	38.400	15.341
	1467	CE	LYS	909	-3.726	38.753	14.996
10	1468	NZ	LYS	909	-4.024	40.246	15.095
	1469	C	LYS	909	0.691	35.136	13.480
	1470	O	LYS	909	0.116	34.647	12.495
	1471	N	CYS	910	1.915	35.660	13.446
15	1472	CA	CYS	910	2.776	35.795	12.272
	1473	CB	CYS	910	4.202	36.113	12.754
	1474	C	CYS	910	2.826	34.582	11.379
20	1475	O	CYS	910	2.789	34.651	10.145
	1476	SG	CYS	910	5.286	36.472	11.353
	1477	N	PRO	911	2.903	33.447	12.024
	1478	CA	PRO	911	3.037	32.243	11.278
25	1479	CB	PRO	911	4.386	31.672	11.628
	1480	C	PRO	911	1.964	31.280	11.628
	1481	O	PRO	911	1.200	31.466	12.578
30	1482	CG	PRO	911	4.509	32.104	13.099
	1483	CD	PRO	911	3.955	33.532	13.103
	1484	N	ASN	912	1.895	30.246	10.817
	1485	CA	ASN	912	0.954	29.196	11.077
35	1486	C	ASN	912	1.861	28.138	11.671
	1487	O	ASN	912	1.440	27.332	12.495
	1488	CB	ASN	912	0.341	28.704	9.733
40	1489	CG	ASN	912	-0.357	29.755	8.863
	1490	OD1	ASN	912	0.187	30.262	7.893
	1491	ND2	ASN	912	-1.563	30.137	9.183
	1492	N	ASN	913	3.134	28.197	11.271
45	1493	CA	ASN	913	4.193	27.258	11.668
	1494	CB	ASN	913	5.251	27.272	10.578
	1495	CG	ASN	913	5.578	28.679	10.136
50	1496	OD1	ASN	913	5.923	29.526	10.956
	1497	ND2	ASN	913	5.420	28.980	8.768
	1498	C	ASN	913	4.881	27.454	13.028
	1499	O	ASN	913	5.908	28.132	13.127
55	1500	N	SER	914	4.332	26.802	14.050
	1501	CA	SER	914	4.830	26.870	15.426

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1502	CB	SER	914	3.756	26.337	16.382
	1503	OG	SER	914	2.498	26.998	16.259
10	1504	C	SER	914	6.140	26.111	15.661
	1505	O	SER	914	6.533	25.861	16.805
	1506	N	GLY	915	6.809	25.755	14.570
	1507	CA	GLY	915	8.074	25.033	14.645
15	1508	C	GLY	915	9.212	25.966	15.088
	1509	O	GLY	915	10.036	25.590	15.933
	1510	N	GLN	916	9.250	27.176	14.526
20	1511	CA	GLN	916	10.278	28.152	14.888
	1512	CB	GLN	916	11.054	28.617	13.646
	1513	CG	GLN	916	12.152	27.631	13.218
	1514	CD	GLN	916	13.209	28.248	12.312
25	1515	OE1	GLN	916	14.225	27.615	12.008
	1516	NE2	GLN	916	12.971	29.540	11.787
	1517	C	GLN	916	9.721	29.356	15.658
30	1518	O	GLN	916	10.144	30.502	15.463
	1519	N	SER	917	8.766	29.074	16.541
	1520	CA	SER	917	8.176	30.109	17.363
	1521	CB	SER	917	6.870	29.626	17.987
35	1522	C	SER	917	9.183	30.515	18.428
	1523	O	SER	917	9.504	31.695	18.551
	1524	OG	SER	917	7.069	28.618	18.985
40	1525	N	TRP	918	9.706	29.564	19.191
	1526	CA	TRP	918	10.703	29.976	20.171
	1527	CB	TRP	918	11.036	28.870	21.173
	1528	CG	TRP	918	9.927	28.533	22.068
45	1529	CD2	TRP	918	9.500	29.264	23.223
	1530	CE2	TRP	918	8.375	28.589	23.743
	1531	CE3	TRP	918	9.997	30.377	23.915
50	1532	CD1	TRP	918	9.049	27.515	21.909
	1533	NE1	TRP	918	8.105	27.543	22.904
	1534	CZ2	TRP	918	7.679	29.048	24.864
	1535	CZ3	TRP	918	9.310	30.830	25.041
55	1536	CH2	TRP	918	8.179	30.144	25.521
	1537	C	TRP	918	11.992	30.412	19.490

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1538	O	TRP	918	12.819	31.066	20.124
	1539	N	GLN	919	12.196	30.066	18.225
10	1540	CA	GLN	919	13.434	30.506	17.602
	1541	CB	GLN	919	13.751	29.719	16.327
	1542	CG	GLN	919	15.178	29.976	15.774
	1543	CD	GLN	919	16.294	29.818	16.827
15	1544	OE1	GLN	919	16.925	30.802	17.240
	1545	NE2	GLN	919	16.541	28.501	17.267
	1546	C	GLN	919	13.363	31.996	17.296
20	1547	O	GLN	919	14.341	32.711	17.482
	1548	N	ARG	920	12.196	32.462	16.855
	1549	CA	ARG	920	12.005	33.878	16.529
	1550	CB	ARG	920	10.734	34.075	15.714
25	1551	CG	ARG	920	10.632	35.476	15.165
	1552	CD	ARG	920	9.499	35.588	14.195
	1553	NE	ARG	920	9.351	36.947	13.680
30	1554	CZ	ARG	920	10.163	37.510	12.794
	1555	NH1	ARG	920	11.233	36.851	12.254
	1556	NH2	ARG	920	9.894	38.785	12.424
	1557	C	ARG	920	11.937	34.762	17.765
35	1558	O	ARG	920	12.311	35.938	17.723
	1559	N	PHE	921	11.434	34.203	18.855
	1560	CA	PHE	921	11.348	34.951	20.092
40	1561	CB	PHE	921	10.608	34.150	21.146
	1562	CG	PHE	921	10.407	34.891	22.422
	1563	CD1	PHE	921	9.321	35.745	22.576
	1564	CD2	PHE	921	11.319	34.774	23.458
45	1565	CE1	PHE	921	9.140	36.456	23.747
	1566	CE2	PHE	921	11.152	35.483	24.639
	1567	CZ	PHE	921	10.062	36.330	24.784
50	1568	C	PHE	921	12.770	35.210	20.568
	1569	O	PHE	921	13.050	36.218	21.215
	1570	N	TYR	922	13.662	34.277	20.237
	1571	CA	TYR	922	15.065	34.379	20.609
55	1572	CB	TYR	922	15.769	33.040	20.370
	1573	CG	TYR	922	17.233	33.089	20.718

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1574	CD1	TYR	922	17.649	33.208	22.045
	1575	CE1	TYR	922	18.990	33.371	22.367
10	1576	CD2	TYR	922	18.200	33.117	19.719
	1577	CE2	TYR	922	19.542	33.282	20.028
	1578	CZ	TYR	922	19.930	33.410	21.353
	1579	OH	TYR	922	21.264	33.555	21.664
15	1580	C	TYR	922	15.769	35.471	19.806
	1581	O	TYR	922	16.503	36.284	20.368
	1582	N	GLN	923	15.547	35.472	18.494
20	1583	CA	GLN	923	16.146	36.468	17.608
	1584	CB	GLN	923	15.770	36.199	16.141
	1585	CG	GLN	923	16.408	34.952	15.508
	1586	CD	GLN	923	15.943	34.684	14.065
25	1587	OE1	GLN	923	14.740	34.616	13.775
	1588	NE2	GLN	923	16.959	34.451	13.110
	1589	C	GLN	923	15.639	37.849	18.011
30	1590	O	GLN	923	16.413	38.766	18.286
	1591	N	LEU	924	14.322	37.996	18.060
	1592	CA	LEU	924	13.753	39.275	18.415
	1593	CB	LEU	924	12.239	39.179	18.452
35	1594	CG	LEU	924	11.639	38.894	17.090
	1595	CD1	LEU	924	10.143	38.920	17.222
	1596	CD2	LEU	924	12.105	39.929	16.088
40	1597	C	LEU	924	14.234	39.874	19.721
	1598	O	LEU	924	14.514	41.064	19.777
	1599	N	THR	925	14.326	39.063	20.771
	1600	CA	THR	925	14.746	39.581	22.071
45	1601	CB	THR	925	14.343	38.610	23.184
	1602	OG1	THR	925	14.997	37.365	23.094
	1603	CG2	THR	925	12.846	38.297	23.091
50	1604	C	THR	925	16.252	39.851	22.121
	1605	O	THR	925	16.738	40.653	22.938
	1606	N	LYS	926	16.966	39.170	21.224
	1607	CA	LYS	926	18.408	39.302	21.059
55	1608	CB	LYS	926	18.884	38.210	20.087
	1609	CG	LYS	926	20.327	37.729	20.247

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1610	CD	LYS	926	20.583	37.132	21.640
	1611	CE	LYS	926	21.660	37.911	22.436
10	1612	NZ	LYS	926	21.351	39.365	22.780
	1613	C	LYS	926	18.601	40.715	20.459
	1614	O	LYS	926	19.507	41.464	20.846
	1615	N	LEU	927	17.717	41.077	19.525
15	1616	CA	LEU	927	17.748	42.395	18.889
	1617	CB	LEU	927	16.650	42.521	17.825
	1618	CG	LEU	927	16.952	43.492	16.671
20	1619	CD1	LEU	927	15.672	43.904	15.970
	1620	CD2	LEU	927	17.674	44.711	17.194
	1621	C	LEU	927	17.501	43.451	19.959
	1622	O	LEU	927	18.214	44.445	20.041
25	1623	N	LEU	928	16.460	43.234	20.759
	1624	CA	LEU	928	16.108	44.154	21.828
	1625	CB	LEU	928	15.010	43.560	22.699
30	1626	CG	LEU	928	13.624	43.652	22.083
	1627	CD1	LEU	928	12.611 1	43.023	22.996
	1628	CD2	LEU	928	13.294	45.105	21.840
	1629	C	LEU	928	17.312	44.432	22.686
35	1630	O	LEU	928	17.554	45.576	23.080
	1631	N	ASP	929	18.061	43.370	22.975
	1632	CA	ASP	929	19.268	43.466	23.789
40	1633	CB	ASP	929	19.844	42.076	24.061
	1634	CG	ASP	929	19.233	41.406	25.276
	1635	OD1	ASP	929	18.373	42.017	25.955
	1636	OD2	ASP	929	19.631	40.251	25.555
45	1637	C	ASP	929	20.338	44.318	23.110
	1638	O	ASP	929	20.934	45.189	23.739
	1639	N	SER	930	20.588	44.068	21.833
50	1640	CA	SER	930	21.606	44.841	21.147
	1641	CB	SER	930	21.860	44.274	19.748
	1642	OG	SER	930	20.780	44.324	18.832
	1643	C	SER	930	21.253	46.324	21.059
55	1644	O	SER	930	22.043	47.121	20.568
	1645	N	MET	931	20.067	46.710	21.527

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
5	1646	CA	MET	931	19.704	48.121	21.477
	1647	CB	MET	931	18.200	48.329	21.657
	1648	CG	MET	931	17.349	47.940	20.468
10	1649	SD	MET	931	17.684	48.878	18.960
	1650	CE	MET	931	17.557	50.532	19.494
	1651	C	MET	931	20.439	48.873	22.571
15	1652	O	MET	931	20.633	50.084	22.468
	1653	N	HIS	932	20.836	48.177	23.632
	1654	CA	HIS	932	21.571	48.865	24.678
	1655	CB	HIS	932	21.769	47.988	25.927
20	1656	CG	HIS	932	20.521	47.749	26.732
	1657	CD2	HIS	932	19.798	46.617	26.920
	1658	ND1	HIS	932	19.934	48.714	27.513
25	1659	CE1	HIS	932	18.898	48.190	28.159
	1660	NE2	HIS	932	18.798	46.923	27.815
	1661	C	HIS	932	22.927	49.210	24.064
30	1662	O	HIS	932	23.499	50.242	24.386
	1663	N	ASP	933	23.438	48.363	23.168
	1664	CA	ASP	933	24.730	48.640	22.525
	1665	CB	ASP	933	25.262	47.385	21.776
35	1666	C	ASP	933	24.619	49.831	21.578
	1667	O	ASP	933	25.430	50.750	21.640
	1668	CG	ASP	933	26.686	47.474	21.207
40	1669	OD1	ASP	933	26.999	47.013	20.119
	1670	OD2	ASP	933	27.547	48.139	22.035
	1671	N	LEU	934	23.613	49.857	20.716
	1672	CA	LEU	934	23.537	50.986	19.807
45	1673	CB	LEU	934	22.477	50.754	18.709
	1674	C	LEU	934	23.149	52.278	20.522
	1675	O	LEU	934	23.643	53.348	20.158
50	1676	CG	LEU	934	22.732	49.537	17.784
	1677	CD1	LEU	934	21.508	49.360	16.873
	1678	CD2	LEU	934	24.040	49.676	16.975
	1679	N	VAL	935	22.288	52.203	21.533
55	1680	CA	VAL	935	21.926	53.425	22.243
	1681	CB	VAL	935	20.942	53.176	23.392

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1682	CG1	VAL	935	20.838	54.420	24.251
	1683	CG2	VAL	935	19.578	52.840	22.834
10	1684	C	VAL	935	23.198	54.025	22.820
	1685	O	VAL	935	23.482	55.204	22.626
	1686	N	SER	936	23.964	53.210	23.530
	1687	CA	SER	936	25.213	53.684	24.096
15	1688	CB	SER	936	26.126	52.532	24.592
	1689	C	SER	936	25.962	54.526	23.037
	1690	O	SER	936	26.249	55.702	23.270
20	1691	OG	SER	936	27.299	53.007	25.241
	1692	N	ASP	937	26.245	53.942	21.872
	1693	CA	ASP	937	26.940	54.653	20.786
	1694	CB	ASP	937	27.064	53.786	19.544
25	1695	CG	ASP	937	28.095	52.733	19.691
	1696	OD1	ASP	937	29.205	53.001	20.143
	1697	C	ASP	937	26.250	55.917	20.337
30	1698	O	ASP	937	26.897	56.926	20.066
	1699	OD2	ASP	937	27.576	51.470	19.631
	1700	N	LEU	938	24.939	55.841	20.209
	1701	CA	LEU	938	24.194	56.994	19.767
35	1702	CB	LEU	938	22.745	56.613	19.505
	1703	CG	LEU	938	22.526	55.761	18.258
	1704	CD1	LEU	938	21.053	55.804	17.907
40	1705	CD2	LEU	938	23.359	56.294	17.101
	1706	C	LEU	938	24.278	58.136	20.765
	1707	O	LEU	938	24.502	59.281	20.380
	1708	N	LEU	939	24.128	57.811	22.048
45	1709	CA	LEU	939	24.149	58.797	23.131
	1710	CB	LEU	939	23.652	58.115	24.413
	1711	CG	LEU	939	22.540	58.624	25.350
50	1712	CD1	LEU	939	21.445	59.418	24.648
	1713	CD2	LEU	939	21.956	57.384	26.015
	1714	C	LEU	939	25.495	59.512	23.375
	1715	O	LEU	939	25.512	60.736	23.544
55	1716	N	GLU	940	26.613	58.777	23.399
	1717	CA	GLU	940	27.930	59.403	23.627

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP							
	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
5	1718	CB	GLU	940	29.094	58.382	23.486
	1719	C	GLU	940	28.154	60.548	22.659
	1720	O	GLU	940	28.576	61.643	23.029
10	1721	CG	GLU	940	30.519	58.995	23.561
	1722	CD	GLU	940	30.834	59.804	24.872
	1723	OE1	GLU	940	30.234	59.461	25.896
15	1724	OE2	GLU	940	31.666	60.706	24.729
	1725	N	PHE	941	27.880	60.238	21.398
	1726	CA	PHE	941	28.004	61.147	20.273
	1727	CB	PHE	941	27.702	60.368	19.001
20	1728	CG	PHE	941	28.400	60.835	17.757
	1729	CD1	PHE	941	28.546	62.194	17.467
	1730	CE1	PHE	941	29.203	62.614	16.306
25	1731	CD2	PHE	941	28.923	59.900	16.866
	1732	CE2	PHE	941	29.578	60.293	15.710
	1733	CZ	PHE	941	29.716	61.652	15.428
	1734	C	PHE	941	26.980	62.268	20.405
30	1735	O	PHE	941	27.032	63.260	19.681
	1736	N	CYS	942	26.029	62.091	21.313
	1737	CA	CYS	942	24.983	63.082	21.515
35	1738	CB	CYS	942	23.667	62.395	21.861
	1739	SG	CYS	942	22.249	63.518	22.095
	1740	C	CYS	942	25.364	64.028	22.630
40	1741	O	CYS	942	25.093	65.227	22.560
	1742	N	PHE	943	25.975	63.457	23.665
	1743	CA	PHE	943	26.444	64.211	24.817
	1744	CB	PHE	943	26.870	63.257	25.950
45	1745	CG	PHE	943	25.725	62.493	26.600
	1746	CD1	PHE	943	24.403	62.897	26.446
	1747	CD2	PHE	943	25.992	61.399	27.431
	1748	CE1	PHE	943	23.356	62.227	27.103
50	1749	CE2	PHE	943	24.953	60.720	28.094
	1750	CZ	PHE	943	23.635	61.137	27.930
	1751	C	PHE	943	27.657	65.018	24.331
55	1752	O	PHE	943	27.739	66.230	24.546
	1753	N	TYR	944	28.580	64.328	23.661

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1754	CA	TYR	944	29.792	64.947	23.117
	1755	CB	TYR	944	30.614	64.019	22.183
10	1756	C	TYR	944	29.352	66.200	22.336
	1757	O	TYR	944	29.713	67.316	22.712
	1758	CG	TYR	944	31.628	64.830	21.403
	1759	CD1	TYR	944	32.695	65.534	22.068
15	1760	CD2	TYR	944	31.503	64.959	19.972
	1761	CE1	TYR	944	33.605	66.358	21.317
	1762	CE2	TYR	944	32.419	65.780	19.229
20	1763	CZ	TYR	944	33.480	66.497	19.889
	1764	OH	TYR	944	34.350	67.294	19.176
	1765	N	THR	945	28.287	66.230	21.337
	1766	CA	THR	945	27.800	67.322	20.501
25	1767	C	THR	945	27.089	68.377	21.331
	1768	O	THR	945	27.152	69.566	21.020
	1769	CB	THR	945	26.837	66.791	19.405
30	1770	OG1	THR	945	27.460	65.817	18.573
	1771	CG2	THR	945	26.356	67.912	18.511
	1772	N	PHE	946	26.423	67.928	22.391
	1773	CA	PHE	946	25.684	68.805	23.294
35	1774	C	PHE	946	26.683	69.701	24.034
	1775	O	PHE	946	26.466	70.902	24.160
	1776	CB	PHE	946	24.899	67.961	24.302
40	1777	CG	PHE	946	24.055	68.766	25.255
	1778	CD1	PHE	946	22.905	69.411	24.823
	1779	CD2	PHE	946	24.442	68.901	26.584
	1780	CE1	PHE	946	22.143	70.187	25.697
45	1781	CE2	PHE	946	23.690	69.673	27.468
	1782	CZ	PHE	946	22.537	70.319	27.025
	1783	N	ARG	947	27.770	69.110	24.527
50	1784	CA	ARG	947	28.799	69.887	25.225
	1785	C	ARG	947	29.519	70.858	24.274
	1786	O	ARG	947	29.941	71.947	24.678
	1787	CB	ARG	947	29.802	68.926	25.920
55	1788	CG	ARG	947	30.861	69.622	26.815
	1789	CD	ARG	947	31.844	68.628	27.446

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
1790	NE	ARG	947	32.810	69.389	28.278
1791	CZ	ARG	947	33.806	68.863	28.977
1792	NH1	ARG	947	34.078	67.592	29.025
1793	NH2	ARG	947	34.549	69.668	29.650
1794	N	GLU	948	29.648	70.476	23.005
1795	CA	GLU	948	30.336	71.328	22.034
1796	C	GLU	948	29.348	72.084	21.156
1797	O	GLU	948	29.743	72.682	20.152
1798	CB	GLU	948	31.277	70.432	21.180
1799	CG	GLU	948	32.464	69.730	21.920
1800	CD	GLU	948	33.610	70.599	22.443
1801	OE1	GLU	948	33.987	71.616	21.876
1802	OE2	GLU	948	34.168	70.135	23.595
1803	N	SER	949	28.070	72.071	21.533
1804	CA	SER	949	27.034	72.719	20.729
1805	C	SER	949	27.350	74.132	20.238
1806	O	SER	949	27.131	74.442	19.071
1807	CB	SER	949	25.690	72.711	21.471
1808	OG	SER	949	25.673	73.463	22.684
1809	N	HIS	950	27.863	74.996	21.105
1810	CA	HIS	950	28.165	76.351	20.660
1811	C	HIS	950	29.304	76.341	19.648
1812	O	HIS	950	29.279	77.087	18.665
1813	CB	HIS	950	28.515	77.260	21.850
1814	CG	HIS	950	27.466	77.222	22.923
1815	ND1	HIS	950	26.098	77.400	22.732
1816	CE1	HIS	950	25.669	77.261	24.001
1817	NE2	HIS	950	26.596	77.025	24.969
1818	CD2	HIS	950	27.768	76.999	24.259
1819	N	ALA	951	30.284	75.470	19.863
1820	CA	ALA	951	31.426	75.374	18.965
1821	C	ALA	951	31.055	74.760	17.623
1822	O	ALA	951	31.589	75.140	16.583
1823	CB	ALA	951	32.532	74.549	19.617
1824	N	LEU	952	30.135	73.806	17.654
1825	CA	LEU	952	29.702	73.117	16.446

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1826	C	LEU	952	28.543	73.820	15.762
	1827	O	LEU	952	28.123	73.419	14.680
10	1828	CB	LEU	952	29.305	71.683	16.797
	1829	CG	LEU	952	30.429	70.781	17.301
	1830	CD1	LEU	952	29.852	69.453	17.772
	1831	CD2	LEU	952	31.442	70.567	16.184
15	1832	N	LYS	953	28.044	74.878	16.387
	1833	CA	LYS	953	26.919	75.618	15.851
	1834	C	LYS	953	25.688	74.721	15.769
20	1835	O	LYS	953	24.879	74.855	14.856
	1836	CB	LYS	953	27.275	76.202	14.455
	1837	CG	LYS	953	28.396	77.270	14.502
	1838	CD	LYS	953	28.727	77.915	13.154
25	1839	CE	LYS	953	29.796	78.997	13.360
	1840	NZ	LYS	953	30.242	79.500	12.048
	1841	N	VAL	954	25.548	73.805	16.726
30	1842	CA	VAL	954	24.396	72.901	16.749
	1843	C	VAL	954	23.448	73.310	17.879
	1844	O	VAL	954	23.850	73.383	19.035
	1845	CB	VAL	954	24.841	71.440	16.958
35	1846	CG1	VAL	954	23.611	70.519	17.045
	1847	CG2	VAL	954	25.752	71.000	15.796
	1848	N	GLU	955	22.197	73.600	17.536
40	1849	CA	GLU	955	21.214	73.984	18.537
	1850	C	GLU	955	20.405	72.802	19.068
	1851	O	GLU	955	19.952	71.973	18.288
	1852	CB	GLU	955	20.238	75.010	17.965
45	1853	CG	GLU	955	19.118	75.361	18.944
	1854	CD	GLU	955	18.123	76.367	18.393
	1855	OE1	GLU	955	18.298	76.824	17.240
50	1856	OE2	GLU	955	17.160	76.703	19.123
	1857	N	PHE	956	20.094	72.231	20.212
	1858	CA	PHE	956	19.219	71.221	20.770
	1859	CB	PHE	956	19.929	70.498	21.911
55	1860	CG	PHE	956	20.927	69.468	21.447
	1861	CD1	PHE	956	22.196	69.830	20.999

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1862	CD2	PHE	956	20.607	68.119	21.520
	1863	CE1	PHE	956	23.121	68.857	20.622
10	1864	CE2	PHE	956	21.518	67.143	21.149
	1865	CZ	PHE	956	22.780	67.511	20.716
	1866	C	PHE	956	17.952	71.918	21.259
15	1867	O	PHE	956	18.024	72.911	21.981
	1868	N	PRO	957	16.764	71.402	20.888
	1869	CD	PRO	957	16.416	70.032	20.472
20	1870	CA	PRO	957	15.575	72.103	21.362
	1871	CB	PRO	957	14.447	71.365	20.659
	1872	CG	PRO	957	14.903	69.963	20.757
25	1873	C	PRO	957	15.475	72.040	22.880
	1874	O	PRO	957	16.409	71.607	23.553
	1875	N	ALA	958	14.331	72.467	23.410
30	1876	CA	ALA	958	14.097	72.501	24.852
	1877	CB	ALA	958	12.877	73.367	25.145
	1878	C	ALA	958	13.909	71.138	25.508
35	1879	O	ALA	958	14.633	70.777	26.439
	1880	N	MET	959	12.912	70.398	25.039
	1881	CA	MET	959	12.643	69.079	25.575
40	1882	CB	MET	959	11.709	68.321	24.623
	1883	CG	MET	959	11.377	66.927	25.090
	1884	SD	MET	959	10.899	66.977	26.813
45	1885	CE	MET	959	9.291	67.636	26.628
	1886	C	MET	959	13.970	68.335	25.741
	1887	O	MET	959	14.433	68.125	26.862
50	1888	N	LEU	960	14.579	67.968	24.613
	1889	CA	LEU	960	15.864	67.258	24.563
	1890	CB	LEU	960	16.367	67.174	23.116
55	1891	CG	LEU	960	16.274	65.922	22.248
	1892	CD1	LEU	960	14.839	65.532	21.975
	1893	CD2	LEU	960	16.973	66.214	20.943
55	1894	C	LEU	960	16.935	67.952	25.394
	1895	O	LEU	960	17.790	67.299	26.003
	1896	N	VAL	961	16.902	69.276	25.378
	1897	CA	VAL	961	17.856	70.091	26.120

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1898	CB	VAL	961	17.706	71.666	26.224
	1899	C	VAL	961	17.957	69.563	27.547
10	1900	O	VAL	961	19.039	69.199	28.011
	1901	CG1	VAL	961	18.703	72.407	25.295
	1902	CG2	VAL	961	17.886	72.321	27.621
	1903	N	GLU	962	16.806	69.518	28.210
15	1904	CA	GLU	962	16.651	69.055	29.593
	1905	CB	GLU	962	15.206	69.219	30.010
	1906	CG	GLU	962	14.904	70.411	30.842
20	1907	CD	GLU	962	13.434	70.465	31.145
	1908	OE1	GLU	962	12.721	69.520	30.737
	1909	OE2	GLU	962	12.990	71.440	31.785
	1910	C	GLU	962	17.019	67.610	29.895
25	1911	O	GLU	962	17.672	67.319	30.900
	1912	N	ILE	963	16.530	66.715	29.043
	1913	CA	ILE	963	16.735	65.276	29.160
30	1914	CB	ILE	963	15.854	64.552	28.143
	1915	CG2	ILE	963	15.968	63.057	28.308
	1916	CG1	ILE	963	14.407	64.986	28.335
	1917	CD1	ILE	963	13.573	64.754	27.120
35	1918	C	ILE	963	18.189	64.865	28.960
	1919	O	ILE	963	18.644	63.878	29.547
	1920	N	ILE	964	18.914	65.604	28.115
40	1921	CA	ILE	964	20.324	65.308	27.887
	1922	CB	ILE	964	20.867	65.955	26.563
	1923	CG2	ILE	964	22.384	65.814	26.499
	1924	CG1	ILE	964	20.292	65.222	25.339
45	1925	CD1	ILE	964	20.013	66.096	24.116
	1926	C	ILE	964	21.097	65.825	29.105
	1927	O	ILE	964	21.970	65.128	29.622
50	1928	N	SER	965	20.757	67.031	29.570
	1929	CA	SER	965	21.391	67.626	30.757
	1930	CB	SER	965	20.865	69.070	31.026
	1931	C	SER	965	21.061	66.760	31.975
55	1932	O	SER	965	21.902	66.526	32.844
	1933	OG	SER	965	19.502	69.092	31.464

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
1934	N	ASP	966	19.818	66.295	32.019
1935	CA	ASP	966	19.303	65.434	33.081
1936	CB	ASP	966	17.883	64.988	32.699
1937	CG	ASP	966	17.209	64.126	33.760
1938	OD1	ASP	966	17.765	63.130	34.230
1939	C	ASP	966	20.211	64.210	33.212
1940	O	ASP	966	20.949	64.053	34.184
1941	OD2	ASP	966	16.115	64.728	34.317
1942	N	GLN	967	20.139	63.372	32.187
1943	CA	GLN	967	20.858	62.106	32.055
1944	CB	GLN	967	20.407	61.462	30.754
1945	CG	GLN	967	18.958	61.134	30.781
1946	CD	GLN	967	18.665	60.195	31.918
1947	OE1	GLN	967	18.006	60.557	32.892
1948	NE2	GLN	967	19.196	58.911	31.958
1949	C	GLN	967	22.379	62.075	32.087
1950	O	GLN	967	22.987	61.168	32.664
1951	N	LEU	968	22.965	63.066	31.431
1952	CA	LEU	968	24.404	63.194	31.282
1953	CB	LEU	968	24.767	64.662	30.896
1954	C	LEU	968	25.260	62.800	32.495
1955	O	LEU	968	26.306	62.165	32.333
1956	CG	LEU	968	26.255	65.071	30.998
1957	CD1	LEU	968	27.125	64.301	29.982
1958	CD2	LEU	968	26.401	66.600	30.833
1959	N	PRO	969	24.827	63.139	33.720
1960	CD	PRO	969	23.761	64.056	34.147
1961	CA	PRO	969	25.651	62.756	34.869
1962	CB	PRO	969	25.002	63.513	36.025
1963	CG	PRO	969	24.385	64.700	35.350
1964	C	PRO	969	25.669	61.252	35.114
1965	O	PRO	969	26.724	60.620	35.093
1966	N	LYS	970	24.489	60.678	35.323
1967	CA	LYS	970	24.382	59.253	35.612
1968	CB	LYS	970	23.093	58.967	36.395
1969	CG	LYS	970	21.918	58.557	35.516

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	1970	CD	LYS	970	20.970	59.705	35.241
	1971	CE	LYS	970	19.993	59.845	36.399
10	1972	NZ	LYS	970	18.955	60.941	36.202
	1973	C	LYS	970	24.465	58.260	34.443
	1974	O	LYS	970	24.428	57.052	34.683
	1975	N	VAL	971	24.557	58.730	33.195
15	1976	CA	VAL	971	24.646	57.790	32.064
	1977	CB	VAL	971	24.076	58.386	30.763
	1978	C	VAL	971	26.088	57.388	31.819
20	1979	O	VAL	971	26.434	56.940	30.727
	1980	CG1	VAL	971	22.556	58.673	30.818
	1981	CG2	VAL	971	24.289	57.551	29.471
	1982	N	GLU	972	26.913	57.538	32.852
25	1983	CA	GLU	972	28.335	57.225	32.772
	1984	CB	GLU	972	29.130	58.508	32.516
	1985	C	GLU	972	28.875	56.589	34.050
30	1986	O	GLU	972	29.789	55.764	34.002
	1987	CG	GLU	972	29.130	59.589	33.646
	1988	CD	GLU	972	29.832	60.922	33.377
	1989	OE1	GLU	972	29.856	61.838	34.188
35	1990	OE2	GLU	972	30.426	60.991	32.153
	1991	N	SER	973	28.308	56.988	35.189
	1992	CA	SER	973	28.731	56.522	36.514
40	1993	CB	SER	973	28.038	57.356	37.602
	1994	C	SER	973	28.536	55.048	36.864
	1995	O	SER	973	29.487	54.346	37.233
	1996	OG	SER	973	28.513	58.706	37.656
45	1997	N	GLY	974	27.293	54.593	36.770
	1998	CA	GLY	974	26.947	53.226	37.110
	1999	C	GLY	974	25.688	53.370	37.941
50	2000	O	GLY	974	25.613	52.946	39.095
	2001	N	ASN	975	24.696	53.998	37.334
	2002	CA	ASN	975	23.438	54.253	38.004
	2003	CB	ASN	975	23.152	55.769	37.918
55	2004	CG	ASN	975	24.345	56.632	38.410
	2005	OD1	ASN	975	25.508	56.343	38.100

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TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GR α IN COMPLEX WITH FP						
ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
2006	ND2	ASN	975	24.052	57.602	39.400
2007	C	ASN	975	22.307	53.415	37.380
2008	O	ASN	975	21.467	52.864	38.093
2009	N	ALA	976	22.343	53.284	36.050
2010	CA	ALA	976	21.348	52.557	35.245
2011	CB	ALA	976	21.235	53.216	33.853
2012	C	ALA	976	21.560	51.042	35.030
2013	O	ALA	976	22.631	50.601	34.612
2014	N	LYS	977	20.512	50.260	35.283
2015	CA	LYS	977	20.559	48.811	35.128
2016	CB	LYS	977	19.815	48.166	36.285
2017	CG	LYS	977	19.808	46.674	36.278
2018	CD	LYS	977	18.743	46.214	37.234
2019	CE	LYS	977	18.641	44.708	37.259
2020	NZ	LYS	977	17.452	44.172	38.042
2021	C	LYS	977	19.920	48.379	33.808
2022	O	LYS	977	18.698	48.379	33.665
2023	N	PRO	978	20.759	47.994	32.857
2024	CA	PRO	978	20.302	47.585	31.535
2025	CB	PRO	978	21.489	47.759	30.556
2026	C	PRO	978	19.723	46.150	31.515
2027	O	PRO	978	20.467	45.190	31.365
2028	CG	PRO	978	22.674	47.424	31.477
2029	CD	PRO	978	22.310	48.109	32.798
2030	N	LEU	979	18.404	46.005	31.678
2031	CA	LEU	979	17.752	44.683	31.668
2032	CB	LEU	979	16.226	44.819	31.756
2033	CG	LEU	979	15.695	45.767	32.823
2034	CD1	LEU	979	14.170	45.795	32.863
2035	CD2	LEU	979	16.246	45.305	34.139
2036	C	LEU	979	18.084	43.939	30.374
2037	O	LEU	979	18.209	44.559	29.320
2038	N	TYR	980	18.217	42.619	30.438
2039	CA	TYR	980	18.517	41.850	29.230
2040	CB	TYR	980	19.994	41.458	29.180
2041	C	TYR	980	17.684	40.579	29.171

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
5	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
	2042	O	TYR	980	17.437	39.953	30.199
	2043	CG	TYR	980	21.010	42.605	29.135
10	2044	CD1	TYR	980	21.693	42.974	30.299
	2045	CD2	TYR	980	21.256	43.294	27.943
	2046	CE1	TYR	980	22.606	44.024	30.272
	2047	CE2	TYR	980	22.170	44.344	27.920
15	2048	CZ	TYR	980	22.844	44.708	29.082
	2049	OH	TYR	980	23.738	45.741	29.055
	2050	N	PHE	981	17.248	40.207	27.972
20	2051	CA	PHE	981	16.476	38.990	27.793
	2052	CB	PHE	981	15.719	39.019	26.466
	2053	CG	PHE	981	14.478	39.838	26.516
	2054	CD1	PHE	981	13.293	39.284	26.973
25	2055	CD2	PHE	981	14.525	41.204	26.255
	2056	CE1	PHE	981	12.168	40.081	27.180
	2057	CE2	PHE	981	13.408	42.012	26.459
30	2058	CZ	PHE	981	12.228	41.449	26.927
	2059	C	PHE	981	17.465	37.848	27.815
	2060	O	PHE	981	17.124	36.725	28.178
	2061	N	HIS	982	18.705	38.164	27.441
35	2062	CA	HIS	982	19.793	37.189	27.394
	2063	CB	HIS	982	20.119	36.846	25.950
	2064	CG	HIS	982	18.928	36.424	25.171
40	2065	CD2	HIS	982	18.431	36.849	23.989
	2066	ND1	HIS	982	18.030	35.495	25.655
	2067	CE1	HIS	982	17.028	35.374	24.807
	2068	NE2	HIS	982	17.245	36.186	23.786
45	2069	C	HIS	982	21.054	37.669	28.067
	2070	O	HIS	982	21.554	38.757	27.770
	2071	N	ARG	983	21.586	36.847	28.961
50	2072	CA	ARG	983	22.811	37.196	29.655
	2073	CB	ARG	983	22.886	36.464	31.006
	2074	CG	ARG	983	22.124	35.132	31.099
	2075	C	ARG	983	24.076	36.946	28.818
55	2076	O	ARG	983	24.800	37.896	28.521
	2077	CD	ARG	983	22.237	34.496	32.495

TABLE 11 (continued)

TABLE 11 (continued)

THREE-DIMENSIONAL COORDINATES OF MR OBTAINED FROM HOMOLOGY MODELING OF THE CRYSTAL STRUCTURE COORDINATES OF GRα IN COMPLEX WITH FP							
	ATOM	ATOM TYPE	RESIDUE	RESIDUE #	X	Y	Z
5	2078	NE	ARG	983	21.504	33.197	32.517
	2079	CZ	ARG	983	21.405	32.388	33.567
	2080	NH1	ARG	983	20.738	31.285	33.433
10	2081	NH2	ARG	983	21.942	32.642	34.727
	2082	N	LYS	984	24.308	35.693	28.408
	2083	CA	LYS	984	25.503	35.276	27.631
15	2084	CB	LYS	984	25.244	35.274	26.094
	2085	CG	LYS	984	26.211	34.352	25.247
	2086	CD	LYS	984	27.026	35.124	24.164
	2087	CE	LYS	984	27.905	34.230	23.243
20	2088	NZ	LYS	984	29.205	33.731	23.855
	2089	C	LYS	984	26.718	36.154	27.961
	2090	O	LYS	984	26.967	37.154	27.246
25	2091	OXT	LYS	984	27.399	35.837	28.965

[0406] It will be understood that various details of the invention may be changed without departing from the scope of the invention. Furthermore, the foregoing description is for the purpose of illustration only, and not for the purpose of limitation the invention being defined by the claims.

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SEQUENCE LISTING

5 <110> Xu, H Eric
Bledsoe, Randy K
Montana, Valerie G.
10 Stewart, Eugene L.
Lambert, Millard H.

15 <120> STRUCTURE OF A GLUCOCORTICOID RECEPTOR LIGAND BINDING DOMAIN
COMPRISING AN EXPANDED BINDING POCKET AND METHODS EMPLOYING SAME

20 <130> PU4803WO

25 <160> 11

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Ser Val Leu Ala Gln Glu Arg Gly Asp Val Met Asp Phe Tyr Lys Thr
55 20 25 30

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20	tcc tcg ggg gaa aca gac tta aag ctt ttg gaa gaa agc att gca aac Ser Ser Gly Glu Thr Asp Leu Lys Leu Leu Glu Glu Ser Ile Ala Asn 115 120 125	384
25	ctc aat agg tcg acc agt gtt cca gag aac ccc aag agt tca gca tcc Leu Asn Arg Ser Thr Ser Val Pro Glu Asn Pro Lys Ser Ser Ala Ser 130 135 140	432
30	act gct gtg tct gct gcc ccc aca gag aag gag ttt cca aaa act cac Thr Ala Val Ser Ala Ala Pro Thr Glu Lys Glu Phe Pro Lys Thr His 145 150 155 160	480
	tct gat gta tct tca gaa cag caa cat ttg aag ggc cag act ggc acc Ser Asp Val Ser Ser Glu Gln Gln His Leu Lys Gly Gln Thr Gly Thr 165 170 175	528
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40	att ttg cag gat ttg gag ttt tct tct ggg tcc cca ggt aaa gag acg Ile Leu Gln Asp Leu Glu Phe Ser Ser Gly Ser Pro Gly Lys Glu Thr 195 200 205	624
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45	ctt tct cct ctg gcg gga gaa gac gat tca ttc ctt ttg gaa gga aac Leu Ser Pro Leu Ala Gly Glu Asp Asp Ser Phe Leu Leu Glu Gly Asn 225 230 235 240	720
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	Leu	Pro	Gln	Val	Lys	Thr	Glu	Lys	Glu	Asp	Phe	Ile	Glu	Leu	Cys	Thr	
			275					280					285				
5																	
	cct	ggg	gta	att	aag	caa	gag	aaa	ctg	ggc	aca	gtt	tac	tgt	cag	gca	912
	Pro	Gly	Val	Ile	Lys	Gln	Glu	Lys	Leu	Gly	Thr	Val	Tyr	Cys	Gln	Ala	
		290					295					300					
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	agc	ttt	cct	gga	gca	aat	ata	att	ggg	aat	aaa	atg	tct	gcc	att	tct	960
	Ser	Phe	Pro	Gly	Ala	Asn	Ile	Ile	Gly	Asn	Lys	Met	Ser	Ala	Ile	Ser	
	305					310				315					320		
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	Val	His	Gly	Val	Ser	Thr	Ser	Gly	Gly	Gln	Met	Tyr	His	Tyr	Asp	Met	
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	aat	aca	gca	tcc	ctt	tct	caa	cag	cag	gat	cag	aag	cct	att	ttt	aat	1056
	Asn	Thr	Ala	Ser	Leu	Ser	Gln	Gln	Gln	Asp	Gln	Lys	Pro	Ile	Phe	Asn	
				340					345					350			
20																	
	gtc	att	cca	cca	att	ccc	gtt	ggg	tcc	gaa	aat	tgg	aat	agg	tgc	caa	1104
	Val	Ile	Pro	Pro	Ile	Pro	Val	Gly	Ser	Glu	Asn	Trp	Asn	Arg	Cys	Gln	
			355				360						365				
	gga	tct	gga	gat	gac	aac	ttg	act	tct	ctg	ggg	act	ctg	aac	ttc	cct	1152
25	Gly	Ser	Gly	Asp	Asp	Asn	Leu	Thr	Ser	Leu	Gly	Thr	Leu	Asn	Phe	Pro	
		370				375					380						
	ggg	cga	aca	gtt	ttt	tct	aat	ggc	tat	tca	agc	ccc	agc	atg	aga	cca	1200
	Gly	Arg	Thr	Val	Phe	Ser	Asn	Gly	Tyr	Ser	Ser	Pro	Ser	Met	Arg	Pro	
	385				390					395					400		
30																	
	gat	gta	agc	tct	cct	cca	tcc	agc	tcc	tca	aca	gca	aca	aca	gga	cca	1248
	Asp	Val	Ser	Ser	Pro	Pro	Ser	Ser	Ser	Ser	Thr	Ala	Thr	Thr	Gly	Pro	
					405					410					415		
	cct	ccc	aaa	ctc	tgc	ctg	gtg	tgc	tct	gat	gaa	gct	tca	gga	tgt	cat	1296
35	Pro	Pro	Lys	Leu	Cys	Leu	Val	Cys	Ser	Asp	Glu	Ala	Ser	Gly	Cys	His	
			420					425					430				
	tat	gga	gtc	tta	act	tgt	gga	agc	tgt	aaa	gtt	ttc	ttc	aaa	aga	gca	1344
	Tyr	Gly	Val	Leu	Thr	Cys	Gly	Ser	Cys	Lys	Val	Phe	Phe	Lys	Arg	Ala	
		435					440					445					
40																	
	gtg	gaa	gga	cag	cac	aat	tac	cta	tgt	gct	gga	agg	aat	gat	tgc	atc	1392
	Val	Glu	Gly	Gln	His	Asn	Tyr	Leu	Cys	Ala	Gly	Arg	Asn	Asp	Cys	Ile	
		450				455					460						
	atc	gat	aaa	att	cga	aga	aaa	aac	tgc	cca	gca	tgc	cgc	tat	cga	aaa	1440
45	Ile	Asp	Lys	Ile	Arg	Arg	Lys	Asn	Cys	Pro	Ala	Cys	Arg	Tyr	Arg	Lys	
	465				470				475						480		
	tgt	ctt	cag	gct	gga	atg	aac	ctg	gaa	gct	cga	aaa	aca	aag	aaa	aaa	1488
	Cys	Leu	Gln	Ala	Gly	Met	Asn	Leu	Glu	Ala	Arg	Lys	Thr	Lys	Lys	Lys	
				485				490						495			
50																	
	ata	aaa	gga	att	cag	cag	gcc	act	aca	gga	gtc	tca	caa	gaa	acc	tct	1536
	Ile	Lys	Gly	Ile	Gln	Gln	Ala	Thr	Thr	Gly	Val	Ser	Gln	Glu	Thr	Ser	
			500				505						510				
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25	atg acc cta ctg cag tac tcc tgg atg ttt ctt atg gca ttt gct ctg Met Thr Leu Leu Gln Tyr Ser Trp Met Phe Leu Met Ala Phe Ala Leu 595 600 605	1824		
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45	cag gta tct tat gaa gag tat ctc tgt atg aaa acc tta ctg ctt ctc Gln Val Ser Tyr Glu Glu Tyr Leu Cys Met Lys Thr Leu Leu Leu Leu 660 665 670	2016		
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Phe Pro Lys Gly Ser Val Ser Asn Ala Gln Gln Pro Asp Leu Ser Lys
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Ala Val Ser Leu Ser Met Gly Leu Tyr Met Gly Glu Thr Glu Thr Lys
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Ser Ser Gly Glu Thr Asp Leu Lys Leu Leu Glu Glu Ser Ile Ala Asn
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Leu Asn Arg Ser Thr Ser Val Pro Glu Asn Pro Lys Ser Ser Ala Ser
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	Ser Asn Glu Asp Cys Lys Pro Leu Ile Leu Pro Asp Thr Lys Pro Lys 245 250 255		
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 Ile Lys Gly Ile Gln Gln Ala Thr Thr Gly Val Ser Gln Glu Thr Ser
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 545 550 555 560
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 565 570 575
 Trp Ala Lys Ala Ile Pro Gly Phe Arg Asn Leu His Leu Asp Asp Gln
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 Met Thr Leu Leu Gln Tyr Ser Trp Met Phe Leu Met Ala Phe Ala Leu
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 610 615 620
 Pro Asp Leu Ile Ile Asn Glu Gln Arg Met Thr Leu Pro Cys Met Tyr
 625 630 635 640
 Asp Gln Cys Lys His Met Leu Tyr Val Ser Ser Glu Leu His Arg Leu
 645 650 655
 45 Gln Val Ser Tyr Glu Glu Tyr Leu Cys Met Lys Thr Leu Leu Leu Leu
 660 665 670
 Ser Ser Val Pro Lys Asp Gly Leu Lys Ser Gln Glu Leu Phe Asp Glu
 675 680 685
 50 Ile Arg Met Thr Tyr Ile Lys Glu Leu Gly Lys Ala Ile Val Lys Arg
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	Leu Ala Glu Ile Ile Thr Asn Gln Ile Pro Lys Tyr Ser Asn Gly Asn		
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	Leu Arg Gly Gly Ala Thr Val Lys Val Ser Ala Ser Ser Pro Ser Leu		
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	Phe Pro Lys Gly Ser Val Ser Asn Ala Gln Gln Pro Asp Leu Ser Lys		
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	Ala Val Ser Leu Ser Met Gly Leu Tyr Met Gly Glu Thr Glu Thr Lys		
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5	tcc tcg ggg gaa aca gac tta aag ctt ttg gaa gaa agc att gca aac	384
	Ser Ser Gly Glu Thr Asp Leu Lys Leu Leu Glu Glu Ser Ile Ala Asn	
	115 120 125	
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	Ser Asn Glu Asp Cys Lys Pro Leu Ile Leu Pro Asp Thr Lys Pro Lys	
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	Ile Lys Asp Asn Gly Asp Leu Val Leu Ser Ser Pro Ser Asn Val Thr	
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	Leu Pro Gln Val Lys Thr Glu Lys Glu Asp Phe Ile Glu Leu Cys Thr	
	275 280 285	
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	Pro Gly Val Ile Lys Gln Glu Lys Leu Gly Thr Val Tyr Cys Gln Ala	
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	Ser Phe Pro Gly Ala Asn Ile Ile Gly Asn Lys Met Ser Ala Ile Ser	
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70	gtt cat ggt gtg agt acc tct gga gga cag atg tac cac tat gac atg	1008
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	370 375 380	
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	385 390 395 400	
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25	tat gga gtc tta act tgt gga agc tgt aaa gtt ttc ttc aaa aga gca Tyr Gly Val Leu Thr Cys Gly Ser Cys Lys Val Phe Phe Lys Arg Ala	1344
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	gtg gaa gga cag cac aat tac cta tgt gct gga agg aat gat tgc atc Val Glu Gly Gln His Asn Tyr Leu Cys Ala Gly Arg Asn Asp Cys Ile	1392
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30	gaa gga aac tcc agc cag aac tgg cag cgg ttt tat caa ctg aca aaa Glu Gly Asn Ser Ser Gln Asn Trp Gln Arg Phe Tyr Gln Leu Thr Lys 705 710 715 720			2160
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35	ttc caa aca ttt ttg gat aag acc atg agt att gaa ttc ccc gag atg Phe Gln Thr Phe Leu Asp Lys Thr Met Ser Ile Glu Phe Pro Glu Met 740 745 750			2256
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	Ala Val Ala Ser Gln Ser Asp Ser Lys Gln Arg Arg Leu Leu Val Asp	50 55 60
15	Phe Pro Lys Gly Ser Val Ser Asn Ala Gln Gln Pro Asp Leu Ser Lys	65 70 75 80
20	Ala Val Ser Leu Ser Met Gly Leu Tyr Met Gly Glu Thr Glu Thr Lys	85 90 95
	Val Met Gly Asn Asp Leu Gly Phe Pro Gln Gln Gly Gln Ile Ser Leu	100 105 110
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	Ser Asp Val Ser Ser Glu Gln Gln His Leu Lys Gly Gln Thr Gly Thr	165 170 175
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	Ile Leu Gln Asp Leu Glu Phe Ser Ser Gly Ser Pro Gly Lys Glu Thr	195 200 205
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Pro Asp Ser Thr Trp Arg Ile Met Thr Thr Leu Asn Met Leu Gly Gly
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	Gln Arg Phe Tyr Gln Leu Thr Lys Leu Leu Asp Ser Met His Glu Val	
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	Val Ser Ser Glu Leu His Arg Leu Gln Val Ser Tyr Glu Glu Tyr Leu 130 135 140			
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Claims

30

1. A crystalline GR polypeptide complex comprising an expanded binding pocket.

35

2. The polypeptide complex of claim 1, wherein an AF2 helix is located in an active position, and where atoms in residues Met560, Met639, Gln642, Cys643, Met646, and Tyr735 have shifted from their positions in a GR/Dex structure, **characterized by** the atomic structural coordinates of Table 3, by one of a heavy-atom RMS deviation of at least about 0.50 angstroms and by a backbone heavy-atom RMS deviation of at least about 0.35 angstroms.

40

3. The polypeptide complex of claim 1, wherein an AF2 helix is located in an active position, and wherein atoms in residues Met560, Met639, Gln642, Cys643, Met646, and Tyr735 have shifted from their positions in a GR/Dex structure, **characterized by** the atomic structural coordinates of Table 3, so as to increase the volume of the main binding pocket by at least about 5%, compared with a GR/Dex structure **characterized by** the atomic structural coordinates of Table 3.

45

4. The polypeptide complex of claim 1, wherein an AF2 helix is located in an active position, and wherein atoms in and around a ligand binding site have shifted from their positions in a GR/Dex structure, **characterized by** the atomic structural coordinates of Table 3, so as to accommodate, without atomic overlap, a steroidal ligand with 17- α substituents comprising 2-20 atoms.

50

5. The polypeptide complex of claim 1, wherein an AF2 helix is located in an active position, and wherein atoms in and around a ligand binding site have shifted from their positions in a GR/Dex structure, **characterized by** the atomic coordinates of Table 3, so as to accommodate, without atomic overlap, a non-steroidal ligand.

55

6. The polypeptide complex of claim 5, wherein the non-steroidal ligand is selected from the group consisting of benzoxazin-1-one and A-222977.

7. The polypeptide complex of claim 1, wherein an AF2 helix is located in an active position, and wherein atoms in and around a ligand binding site have shifted from their positions in a GR/Dex structure, **characterized by** the atomic coordinates of Table 3, such that fluticasone propionate can be docked into a binding site with a favorable

binding energy and wherein all atoms in the polypeptide are held fixed.

8. The polypeptide complex of claim 7, wherein the non-steroidal ligand is selected from the group consisting of benzoxazin-1-one and A-222977.

9. The polypeptide complex of claim 1, further comprising fluticasone propionate and a co-activator peptide.

10. The polypeptide complex of claim 9, wherein the crystalline form comprises lattice constants of $a = b = 127.656 \text{ \AA}$, $c = 87.725 \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 120^\circ$.

11. The polypeptide complex of claim 9, wherein the co-activator peptide is a TIF2 peptide.

12. The polypeptide complex of claim 9, wherein the complex comprises a hexagonal crystalline form.

13. The polypeptide complex of claim 9, wherein the crystalline form has a space group of $P6_1$.

14. The polypeptide complex of claim 9, wherein the GR polypeptide comprises a GR α ligand binding domain.

15. The polypeptide complex of claim 15, wherein the GR α polypeptide has the amino acid sequence shown in any one of SEQ ID NOs: 6 or 8.

16. The polypeptide complex of claim 15, further **characterized by** the atomic structure coordinates shown in Table 2.

17. The polypeptide complex of claim 15, wherein the crystalline form comprises two GR α ligand binding domain polypeptides in the asymmetric unit.

18. The polypeptide complex of claim 15, wherein the complex is such that the three-dimensional structure of the crystallized GR α ligand binding domain polypeptide can be determined to a resolution of about 3.0 \AA or better.

19. The polypeptide complex of claim 9, wherein the complex comprises one or more atoms having a molecular weight of 40 grams/mol or greater.

20. A method for determining the three-dimensional structure of a crystallized GR polypeptide complex comprising an expanded binding pocket to a resolution of about 3.0 \AA or better, the method comprising:

- (a) crystallizing a GR ligand binding domain polypeptide; and
- (b) analyzing the GR ligand binding domain polypeptide to determine the three-dimensional structure of the crystallized GR ligand binding domain polypeptide, whereby the three-dimensional structure of a crystallized GR polypeptide complex comprising an expanded binding pocket is determined to a resolution of about 3.0 \AA or better.

21. The method of claim 20, wherein the reservoir solution comprises 60mM bis-Tris-propane, pH 7.5-8.5, and 1.5-1.7 M magnesium sulfate.

22. The method of claim 20, wherein the co-activator peptide is a TIF2 peptide.

23. The method of claim 20, wherein the GR ligand binding domain comprises one of SEQ ID NO: 6 and SEQ ID NO: 8.

24. A method of generating a crystallized GR polypeptide complex comprising an expanded binding pocket and a ligand known or suspected to be unable to associate with a known GR structure, the method comprising:

- (a) providing a solution comprising a GR polypeptide and a ligand known or suspected to be unable to associate with a known GR structure; and
- (b) crystallizing the GR ligand binding domain polypeptide using the hanging drop method, whereby a crystallized GR polypeptide complex comprising an expanded binding pocket and a ligand known or suspected to be unable to associate with a known GR structure is generated.

25. The method of claim 24, wherein the solution comprises 475 mM ammonium acetate, 25 mM NaCl, 50 mM Tris, pH 8.0, 10% glycerol, 10 mM dithiothreitol (DTT), 0.5mM EDTA and 0.05% β -octyl-glucoside.

26. The method of claim 24, wherein a crystallization reservoir solution comprises 60mM bis-Tris-propane, pH 7.5-8.5, and 1.5-1.7 M magnesium sulfate.

28. The method of claim 24, wherein the co-activator peptide is a TIF2 peptide.

29. The method of claim 24, wherein the GR polypeptide comprises one of SEQ ID NO: 6 and SEQ ID NO: 8.

30. A method for identifying a GR modulator, the method comprising:

- (a) providing atomic coordinates of a GR polypeptide complex comprising an expanded binding pocket to a computerized modeling system; and
- (b) modeling a ligand that fits spatially into the large pocket volume of the GR polypeptide complex to thereby identify a GR modulator.

31. A method of designing a modulator that selectively modulates the activity of a GR α polypeptide comprising an expanded binding pocket, the method comprising:

- (a) providing a crystalline form of a GR α polypeptide complex comprising an expanded binding pocket;
- (b) determining the three-dimensional structure of the crystalline form of the GR α ligand binding domain polypeptide; and
- (c) synthesizing a modulator based on the three-dimensional structure of the crystalline form of the GR α ligand binding domain polypeptide, whereby a modulator that selectively modulates the activity of a GR α polypeptide comprising an expanded binding pocket is designed.

32. The method of claim 31, wherein the method further comprises contacting a GR α polypeptide with the potential modulator; and assaying the GR α polypeptide for binding of the potential modulator, for a change in activity of the GR α polypeptide, or both.

33. A method of forming a homology model of an NR, the method comprising:

- (a) providing a template amino acid sequence comprising a GR polypeptide comprising an expanded binding pocket;
- (b) providing a target NR amino acid sequence;
- (c) aligning the target sequence and the template sequence to form a homology model.

34. The method of claim 33, further comprising assigning structural coordinates to the homology model.

35. The method of claim 33, wherein the NR is selected from the group consisting of AR, PR, ER, GR and MR.

36. The method of claim 33, wherein the template amino acid sequence comprises one of the atomic coordinates of Table 2 and a subset of the coordinates of Table 2.

37. The method of claim 33, wherein the template amino acid sequence comprises spatial coordinates characterizing an AF2 helix located in an active position, and wherein the spatial coordinates further characterize atoms in residues Met560, Met639, Gln642, Cys643, Met646, and Tyr735 that have shifted from their positions in a GR/Dex structure, **characterized by** the atomic structural coordinates of Table 3, by one of a heavy-atom RMS deviation of at least about 0.50 angstroms and by a backbone heavy-atom RMS deviation of at least about 0.35 angstroms.

38. The method of claim 33, wherein the template amino acid sequence comprises spatial coordinates characterizing an AF2 helix located in an active position, and wherein the spatial coordinates further characterize atoms in residues Met560, Met639, Gln642, Cys643, Met646, and Tyr735 that have shifted from their positions in a GR/Dex structure, **characterized by** the atomic structural coordinates of Table 3, so as to increase the volume of a binding pocket by at least about 5%, compared with a GR/Dex structure **characterized by** the atomic structural coordinates of Table 3.

39. The method of claim 33, wherein the template amino acid sequence comprises spatial coordinates characterizing an AF2 helix located in an active position, and wherein the spatial coordinates further characterize atoms in and around a ligand binding site that have shifted from their positions in a GR/Dex structure, **characterized by** the atomic structural coordinates of Table 3, so as to accommodate, without atomic overlap, a steroidal ligand with C17- α substituents comprising 2-20 atoms.

40. The method of claim 33, wherein the template amino acid sequence comprises spatial coordinates characterizing an AF2 helix located in an active position, and wherein the spatial coordinates further characterize atoms in and around a ligand binding site that have shifted from their positions in a GR/Dex structure, **characterized by** the atomic coordinates of Table 3, so as to accommodate, without atomic overlap, a non-steroidal ligand.

41. The method of claim 33, wherein the template amino acid sequence comprises spatial coordinates characterize an AF2 helix located in an active position, and wherein the spatial coordinates further characterize atoms in and around a ligand binding site that have shifted from their positions in a GR/Dex structure, **characterized by** the atomic coordinates of Table 3, such that fluticasone propionate can be docked into a binding site with a favorable binding energy and wherein all atoms in the polypeptide are held fixed.

42. The method of claim 33, wherein the template amino acid sequence comprises spatial coordinates characterizing an AF2 helix is located in an active position, and wherein the spatial coordinates further characterize atoms in and around the ligand binding site that have shifted from their positions in a GR/Dex structure, **characterized by** the atomic coordinates of Table 3, such that a non-steroidal GR ligand can be docked into the binding site with a favorable binding energy, as computed with molecular modeling software, and wherein all atoms in the polypeptide are held fixed.

43. A method of designing a modulator of a nuclear receptor, the method comprising:

- (a) designing a potential modulator of a nuclear receptor that will make interactions with amino acids in the ligand binding site of the nuclear receptor based upon atomic structure coordinates of a NR polypeptide complex comprising an expanded binding pocket;
- (b) synthesizing the modulator; and
- (c) determining whether the potential modulator modulates the activity of the nuclear receptor, whereby a modulator of a nuclear receptor is designed.

44. The method of claim 46, wherein the potential modulator is a non-steroidal compound.

45. The method of claim 46, wherein the potential modulator is a steroid compound.

46. A method of modeling an interaction between an NR and a non-steroid ligand, the method comprising:

- (a) providing a homology model of a target NR generated using a crystalline GR polypeptide complex comprising an expanded binding pocket;
- (b) providing atomic coordinates of a non-steroid ligand; and
- (c) docking the non-steroid ligand with the homology model to form a NR/ligand model.

47. A method of designing a non-steroid modulator of a target NR using a homology model, the method comprising:

- (a) modeling an interaction between a target NR and a non-steroid ligand using a homology model generated using a crystalline GR polypeptide complex comprising an expanded binding pocket;
- (b) evaluating the interaction between the target NR and the non-steroid ligand to determine a first binding efficiency;
- (c) modifying the structure of the non-steroid ligand to form a modified ligand;
- (d) modeling an interaction between the modified ligand and the target NR;
- (e) evaluating the interaction between the target NR and the modified ligand to determine a second binding efficiency; and
- (f) repeating steps (c)-(e) a desired number of times if the second binding efficiency is less than the first binding efficiency.

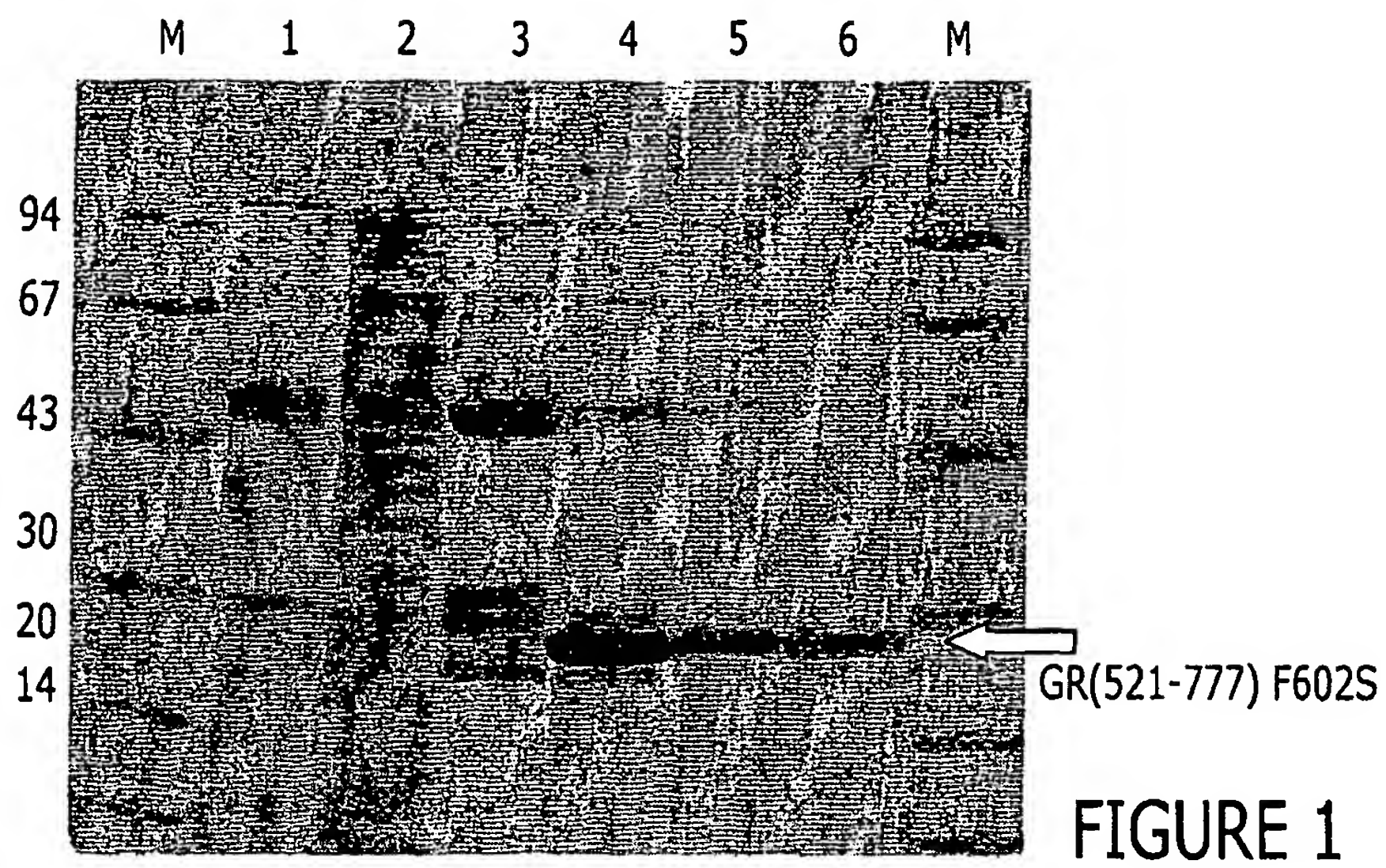


FIGURE 1

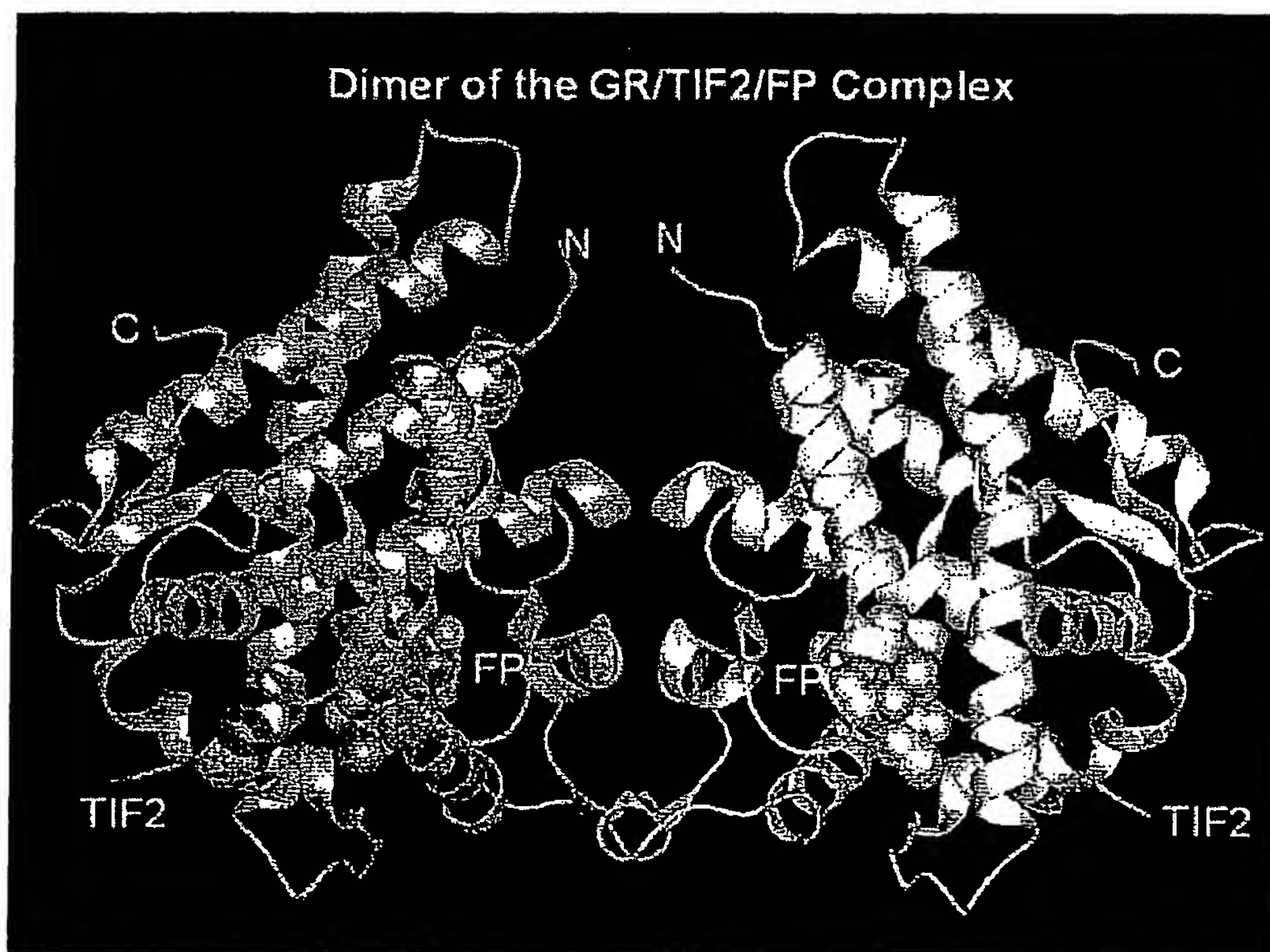


FIGURE 2

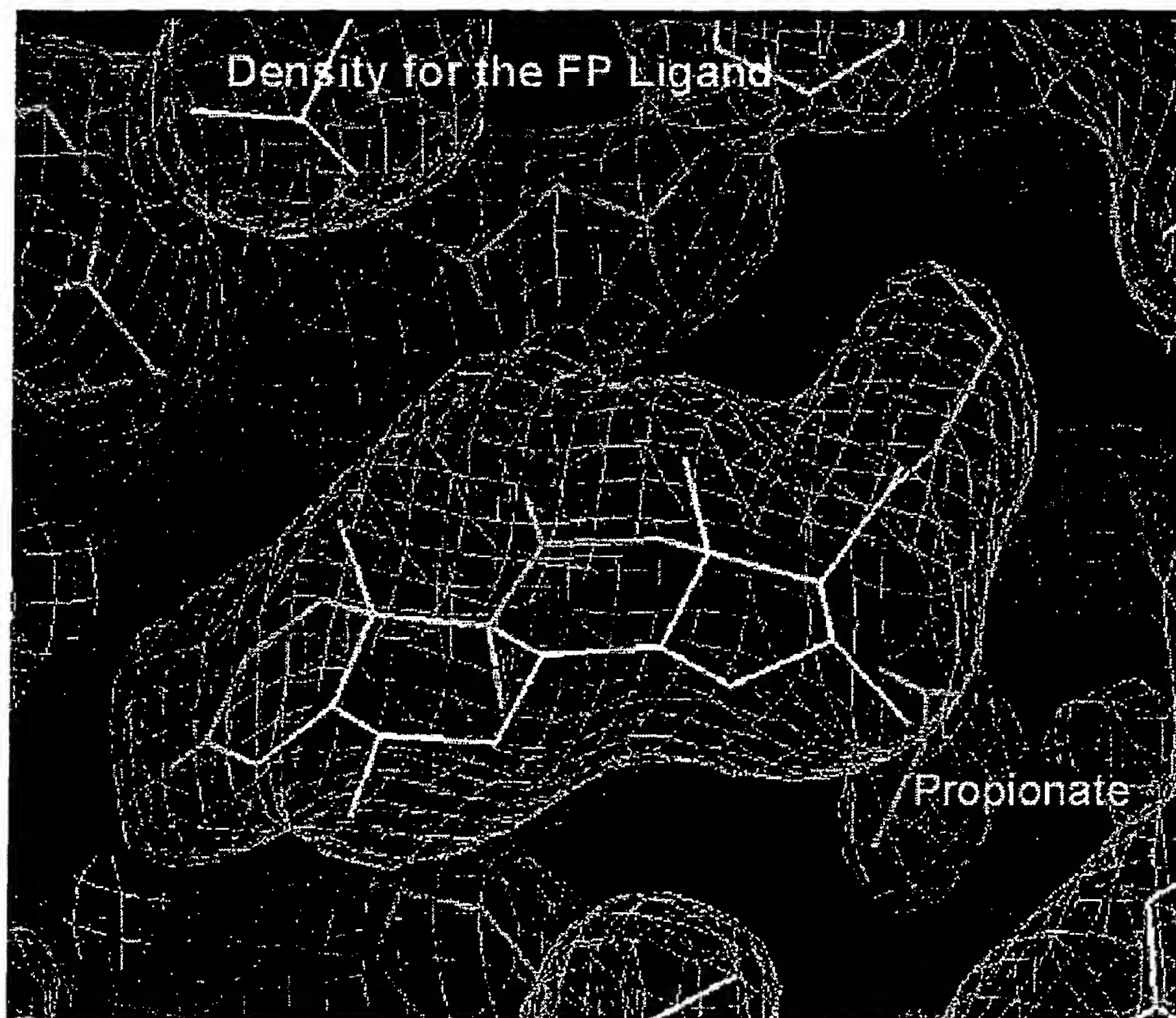


FIGURE 3

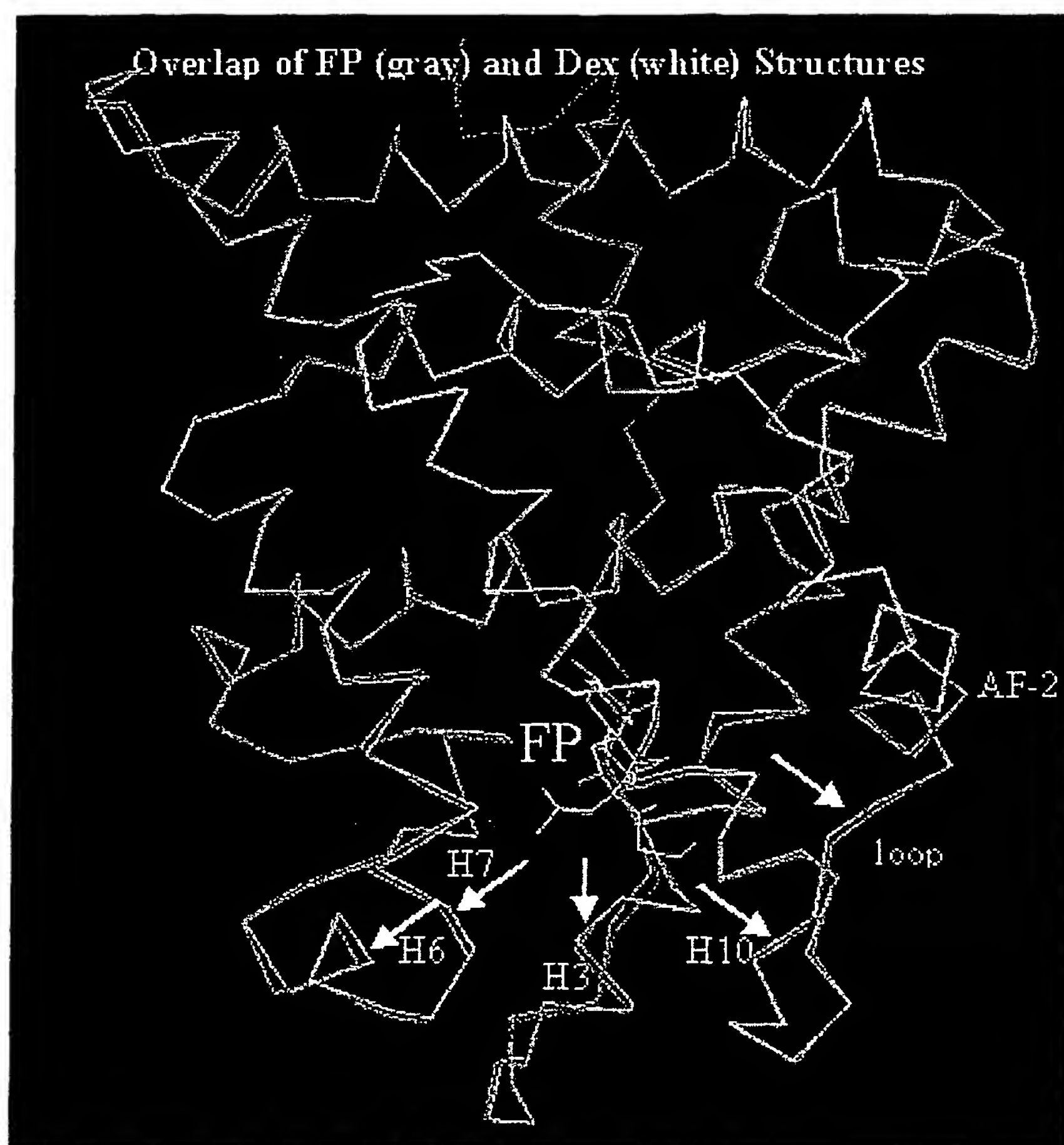


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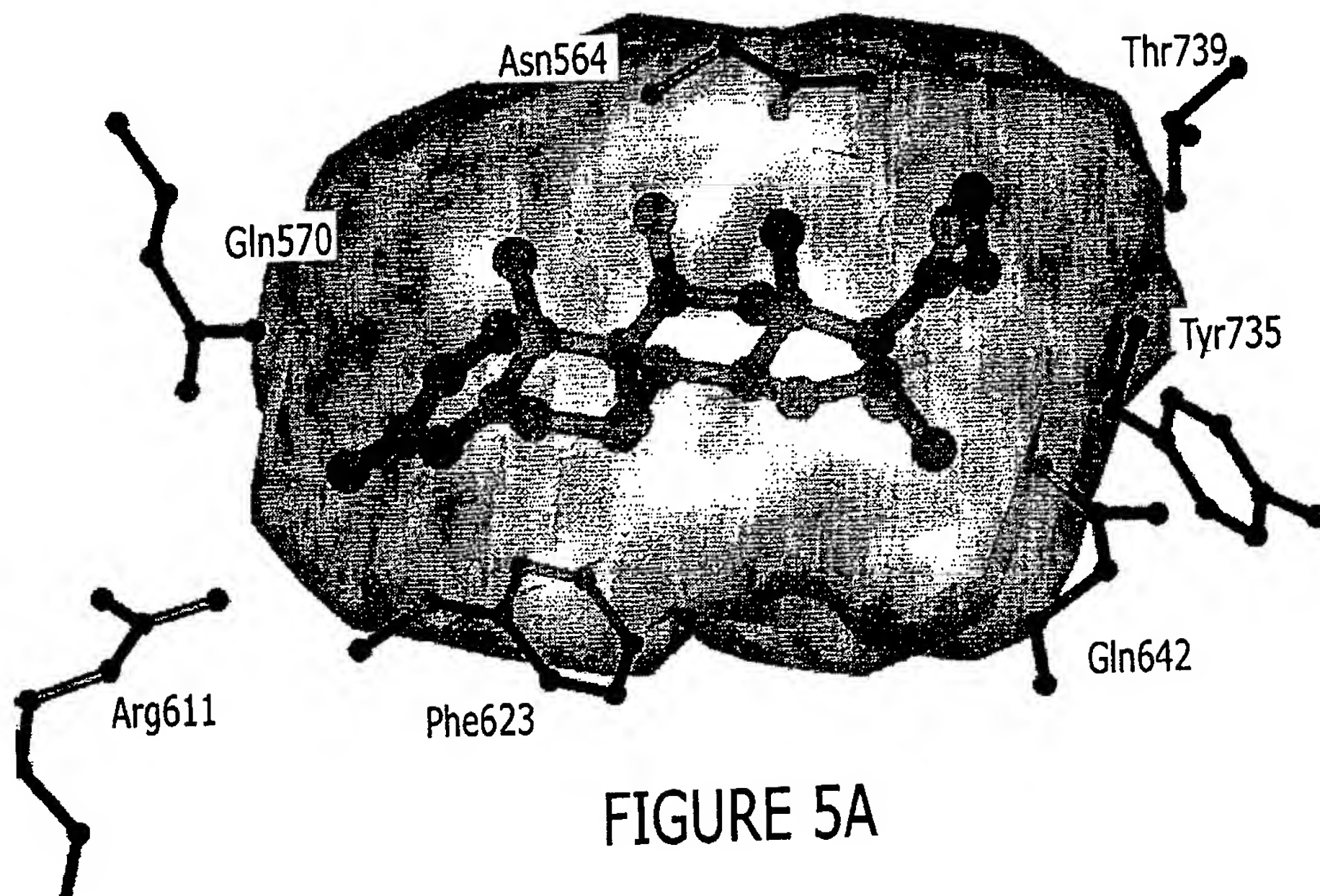


FIGURE 5A

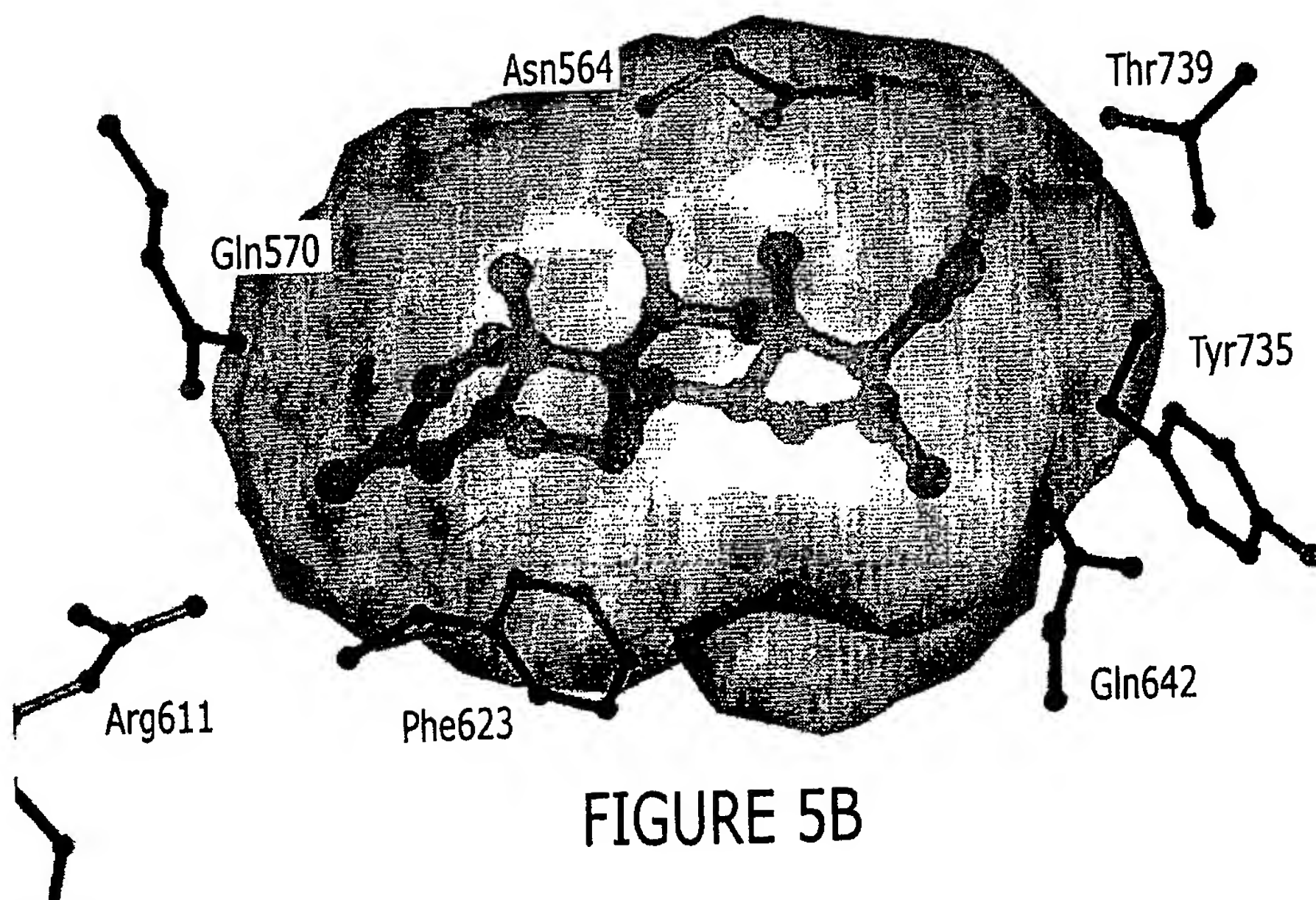


FIGURE 5B

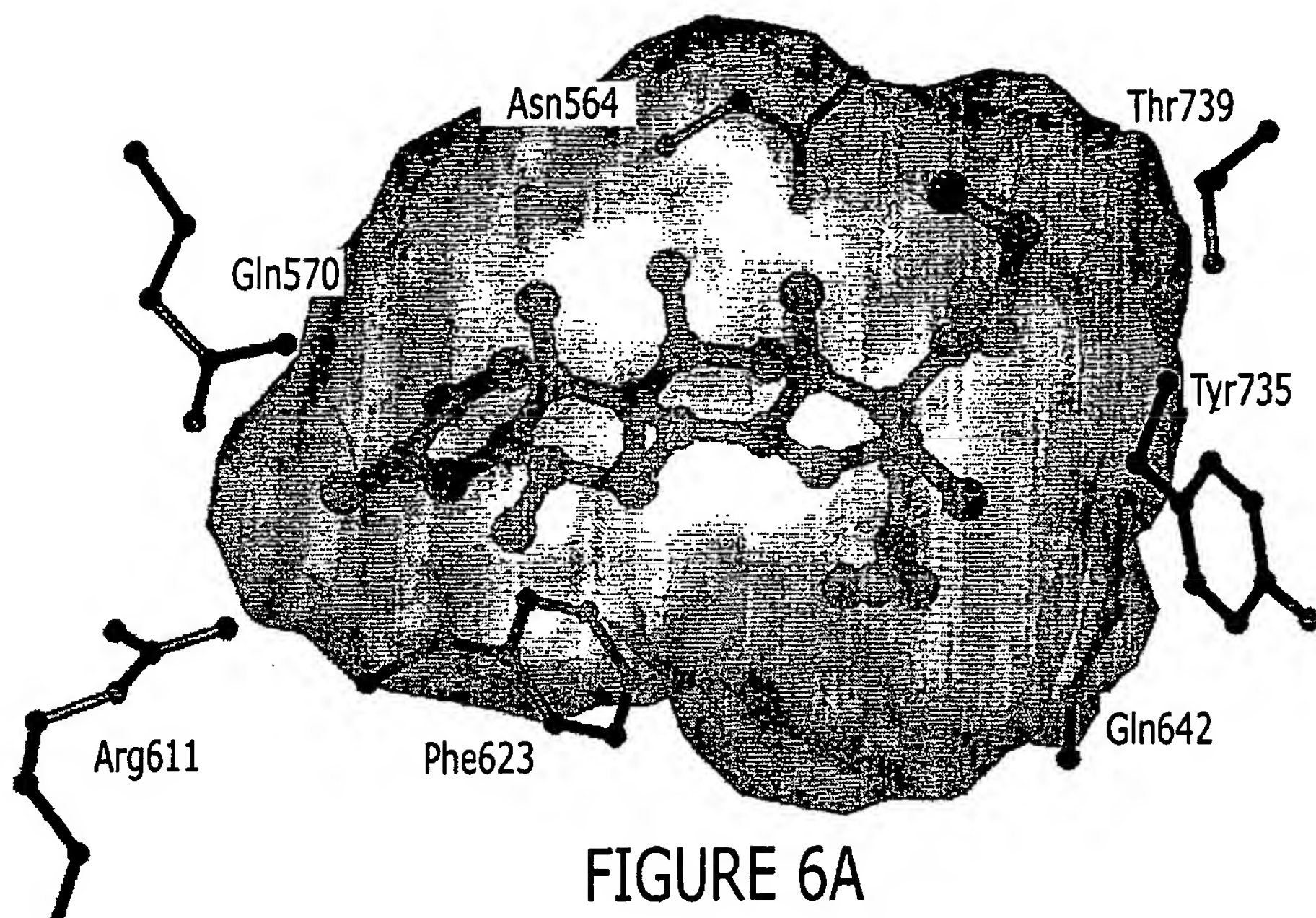


FIGURE 6A

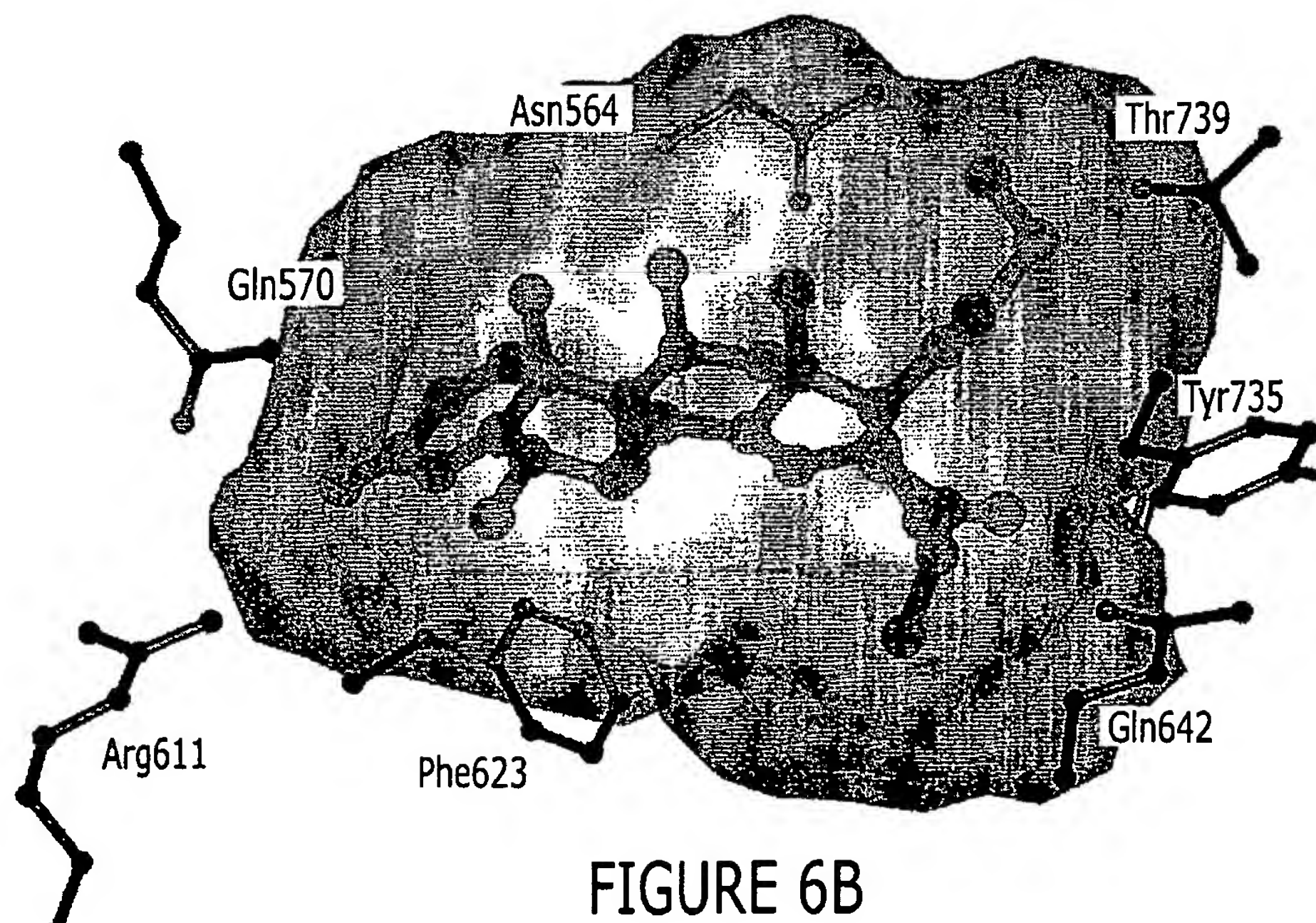


FIGURE 6B

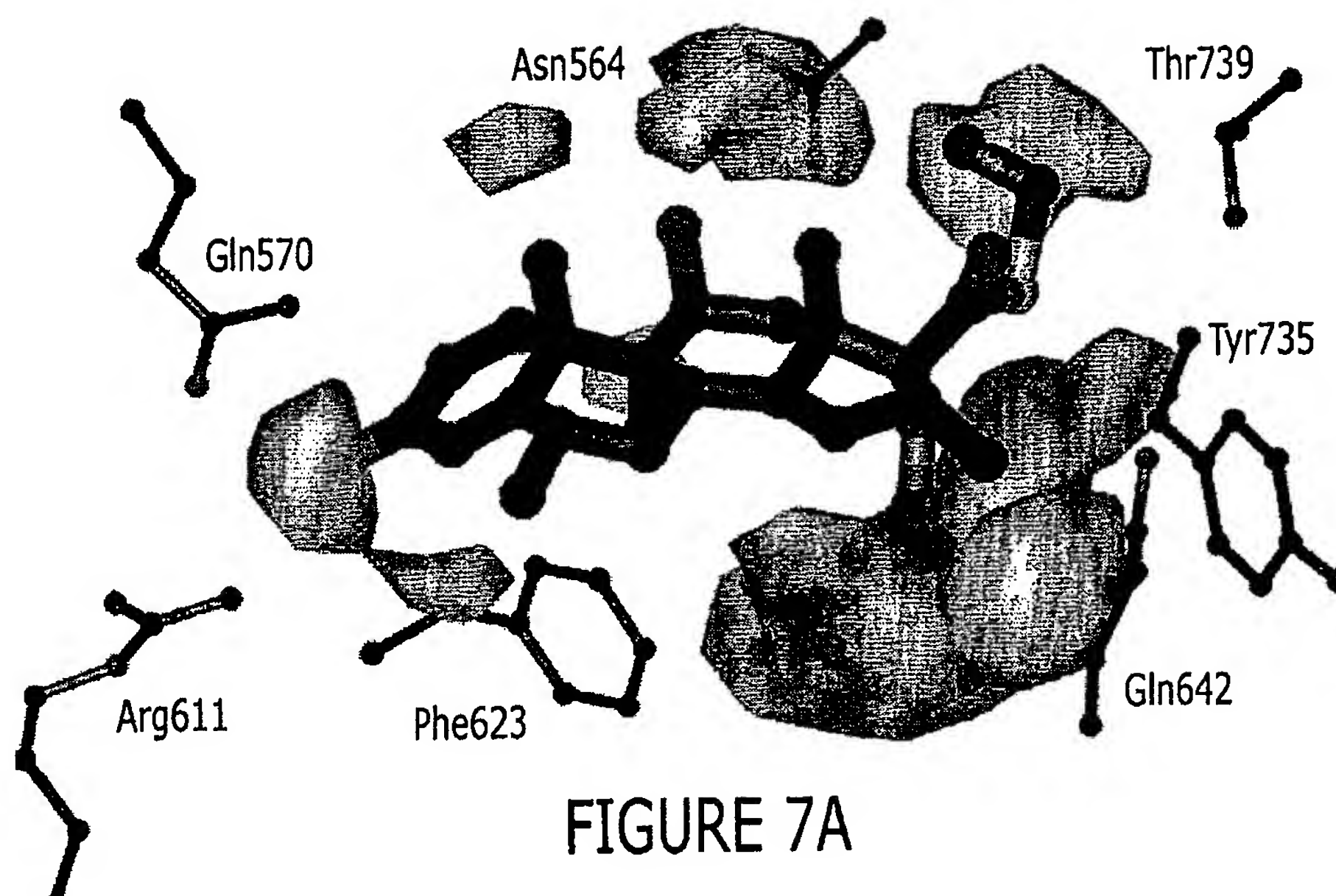


FIGURE 7A

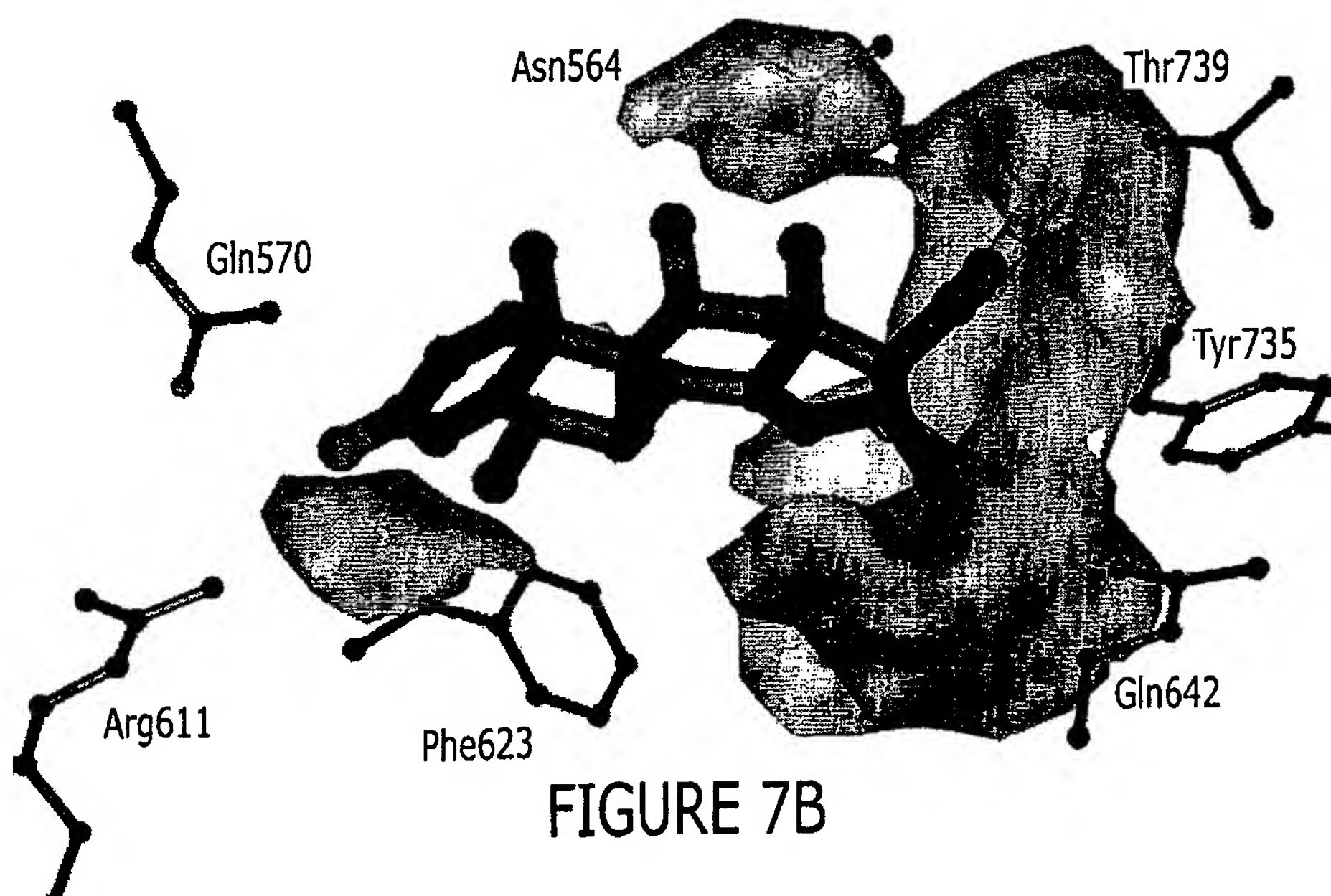
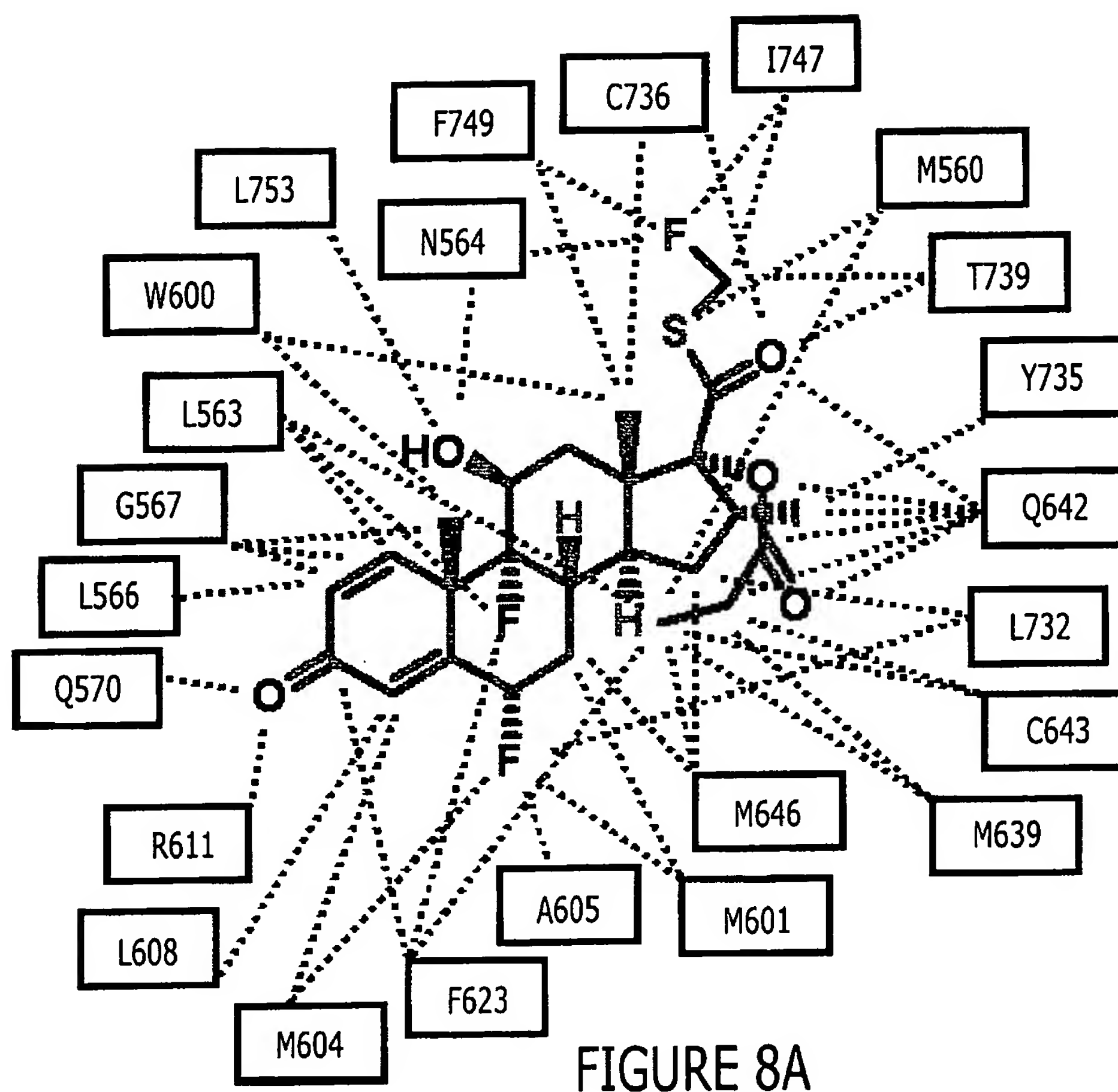


FIGURE 7B



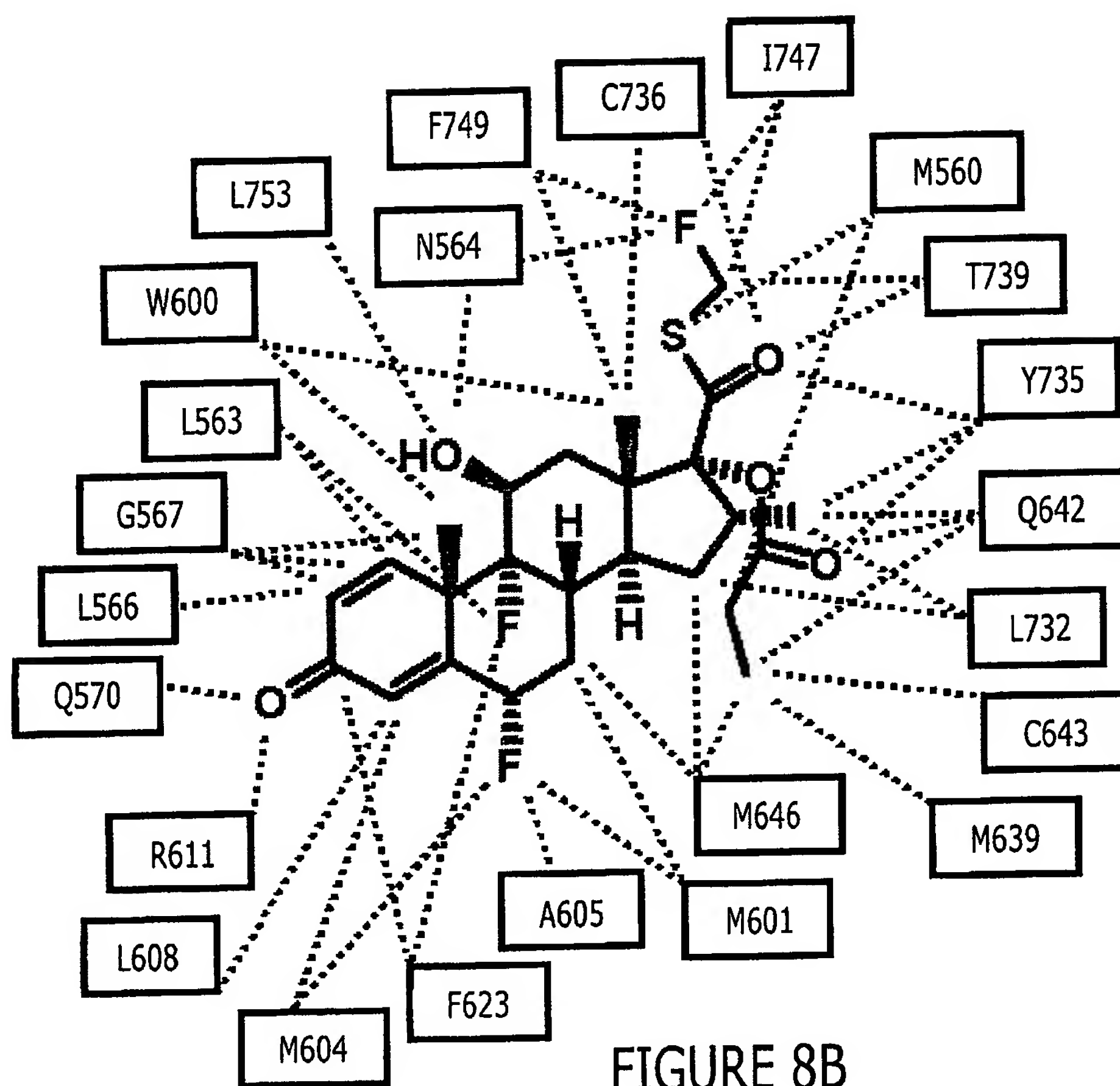


FIGURE 8B

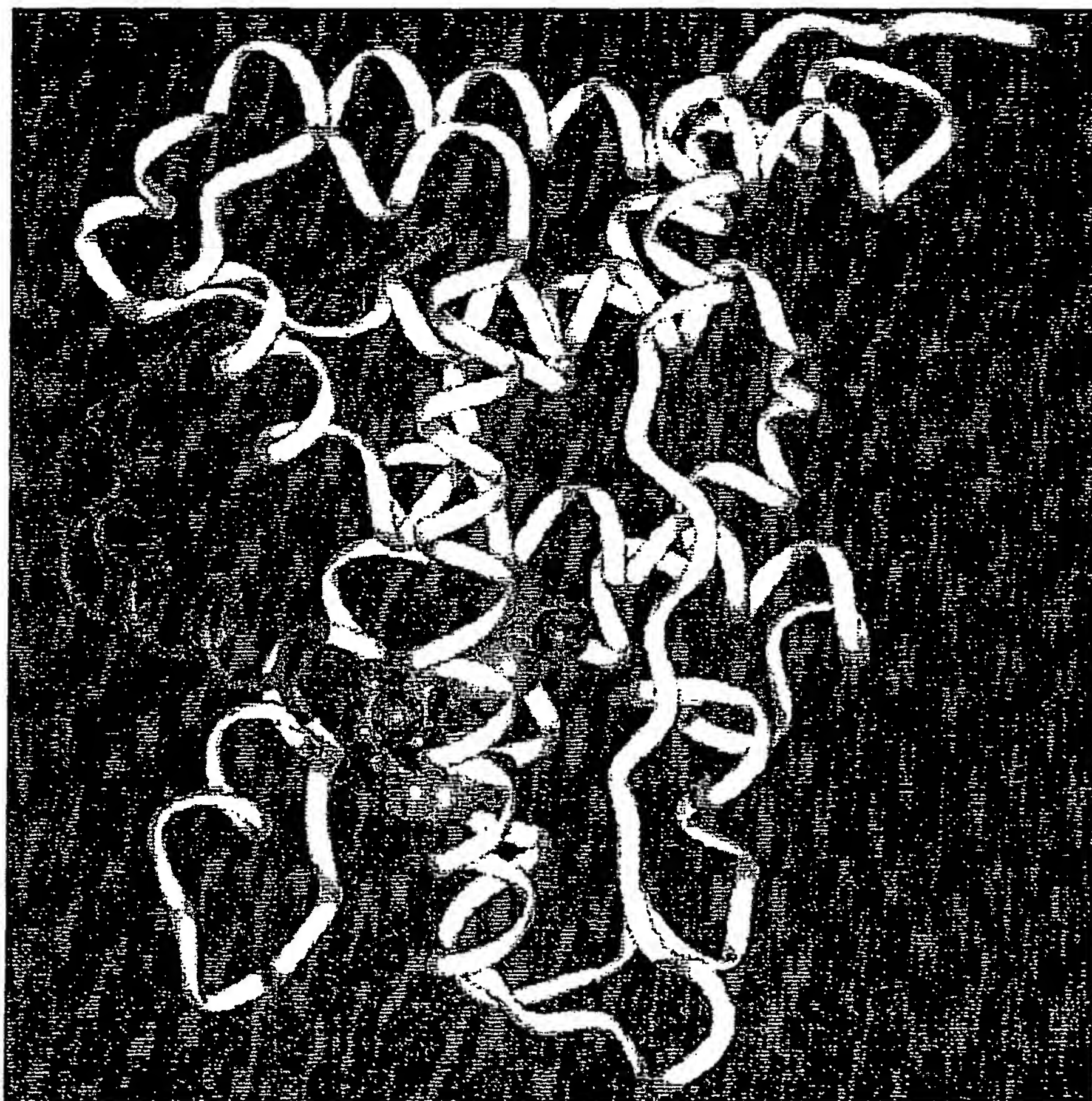


FIGURE 9

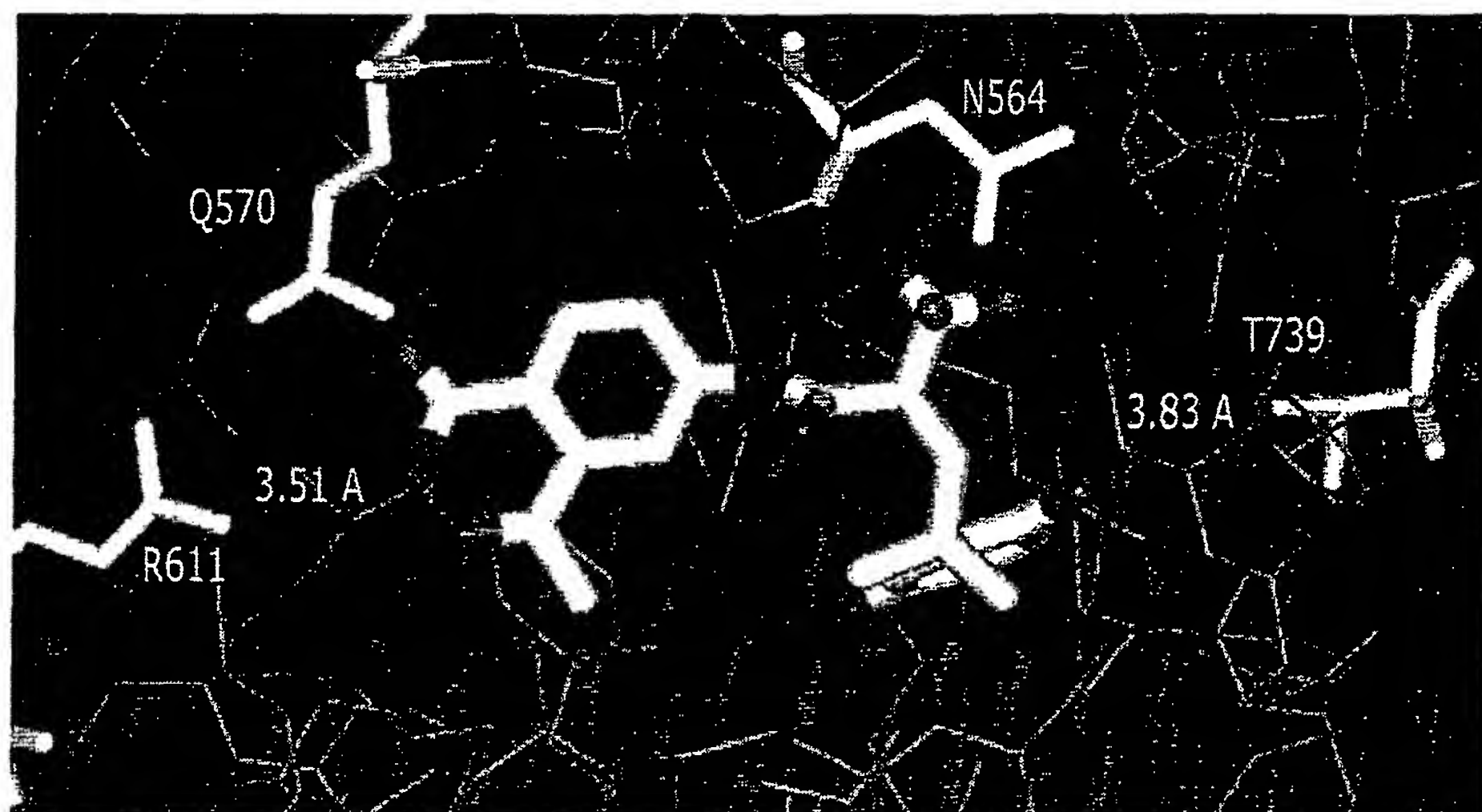


FIGURE 10

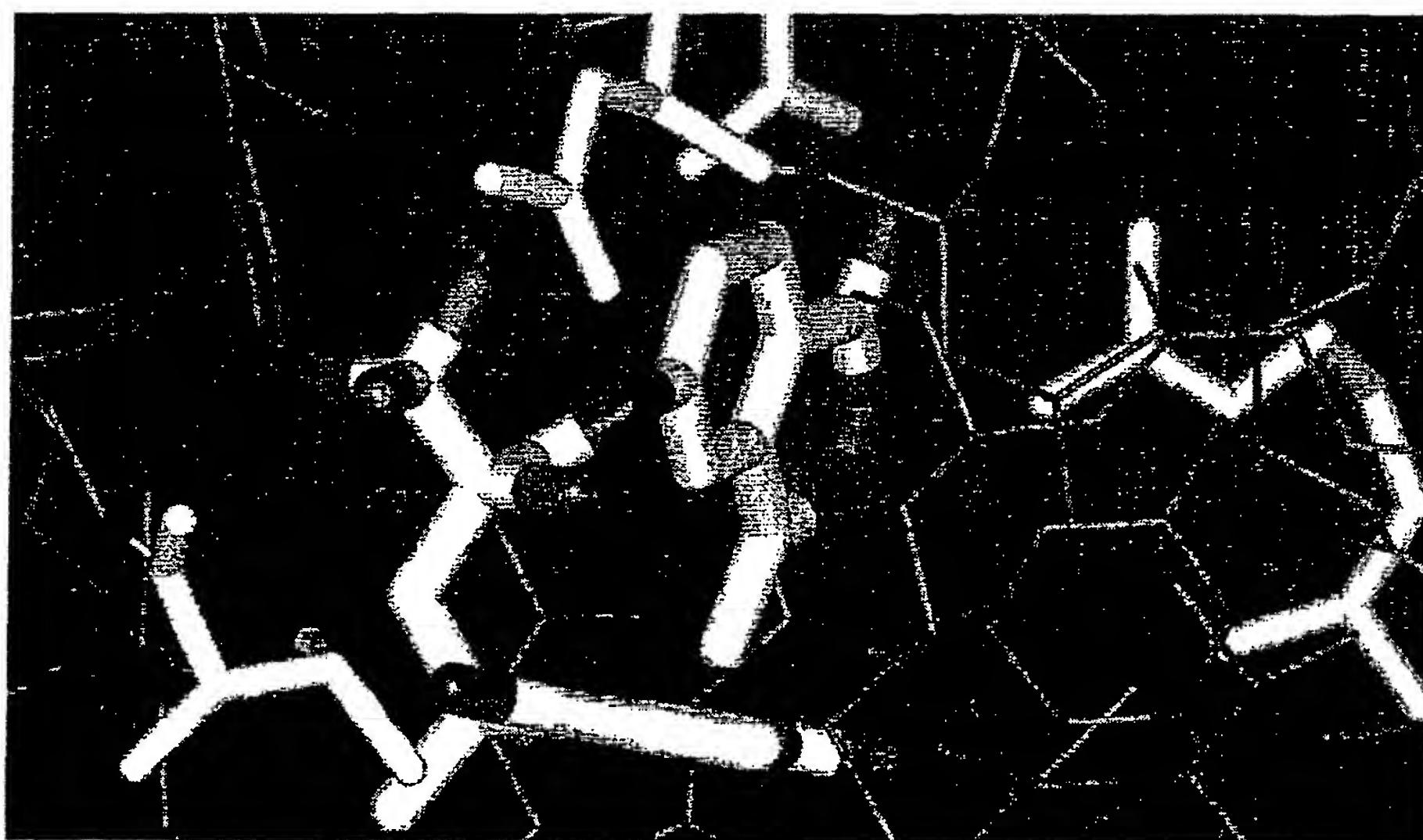


FIGURE 11

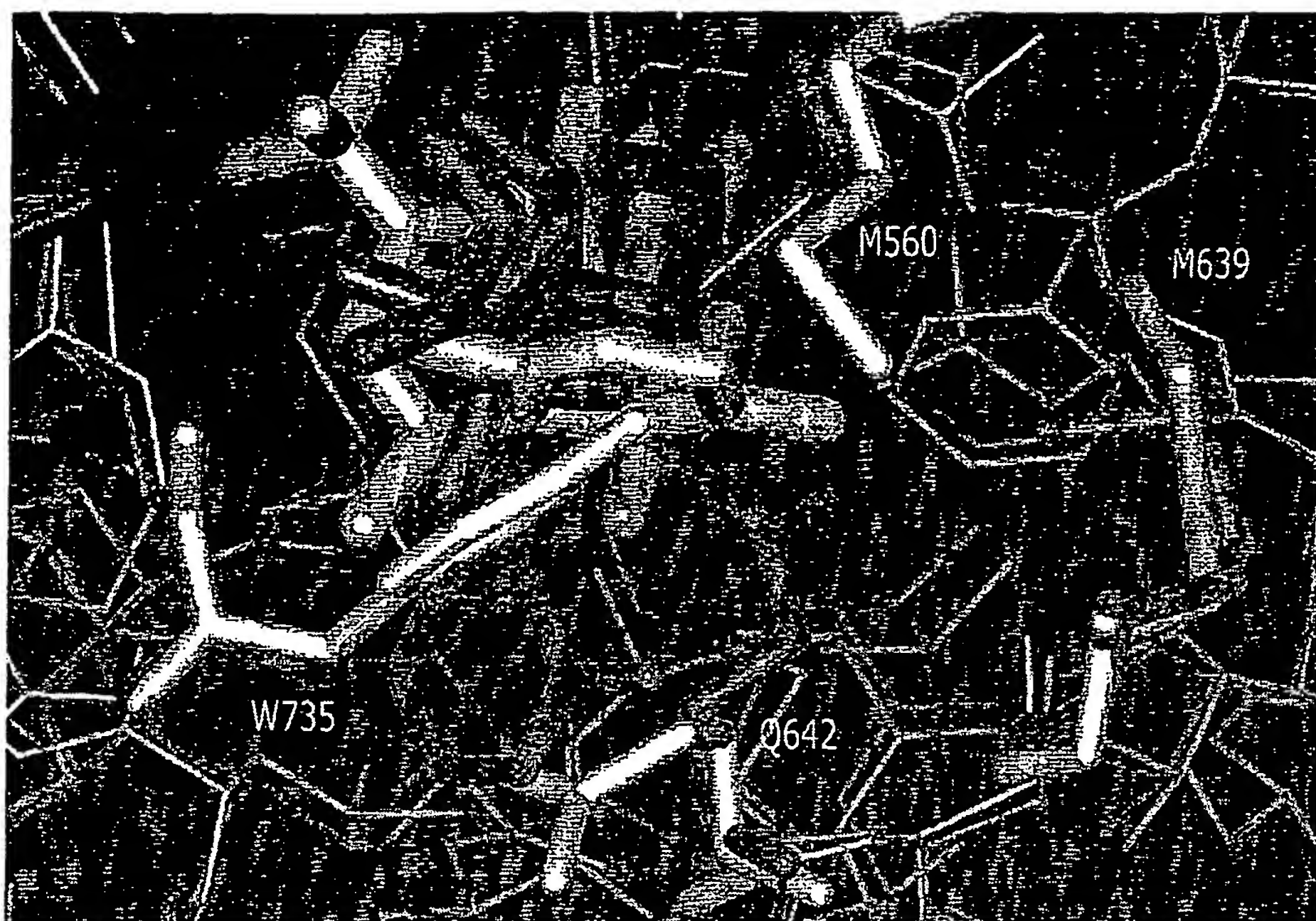


FIGURE 12

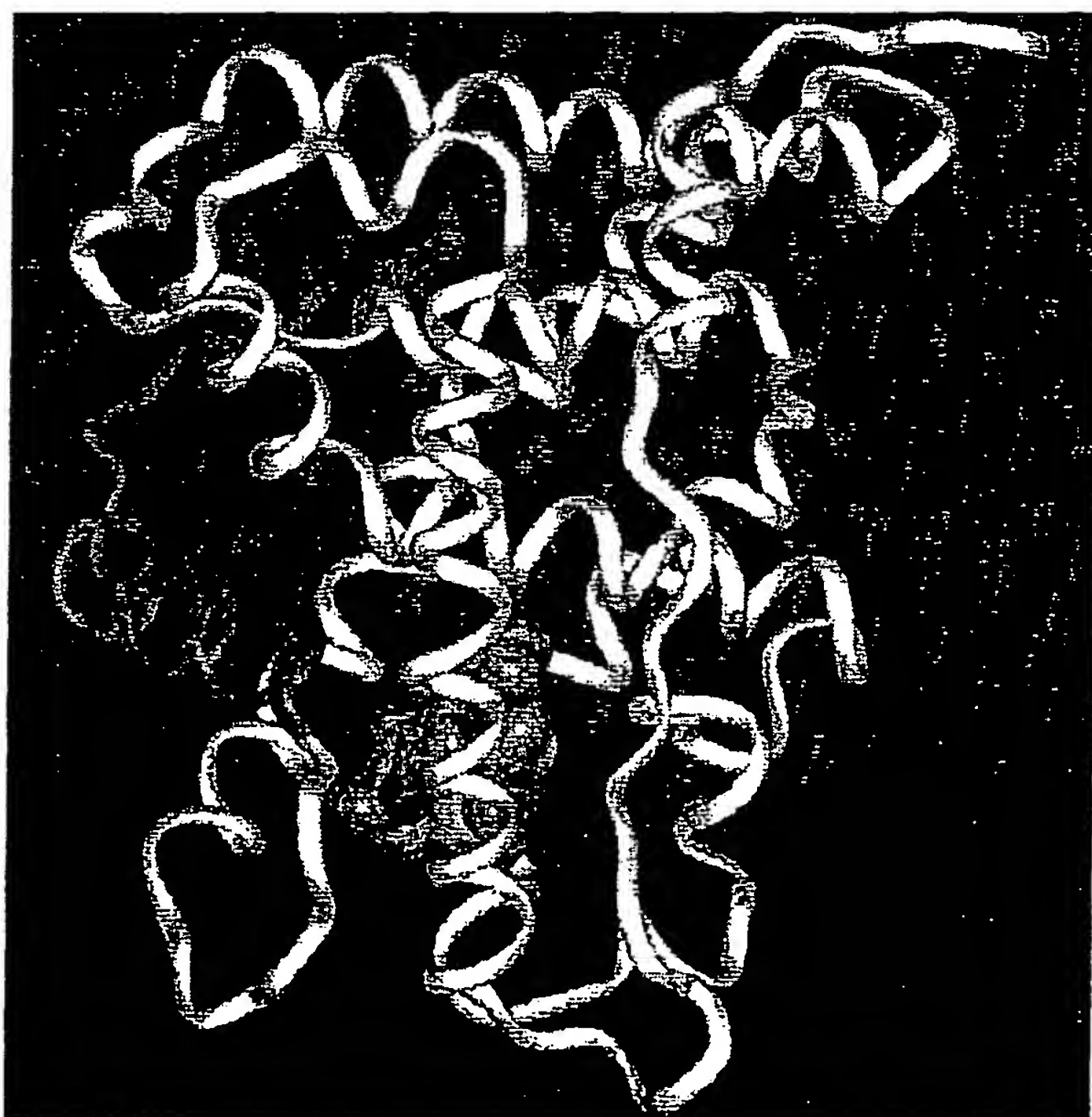


FIGURE 13

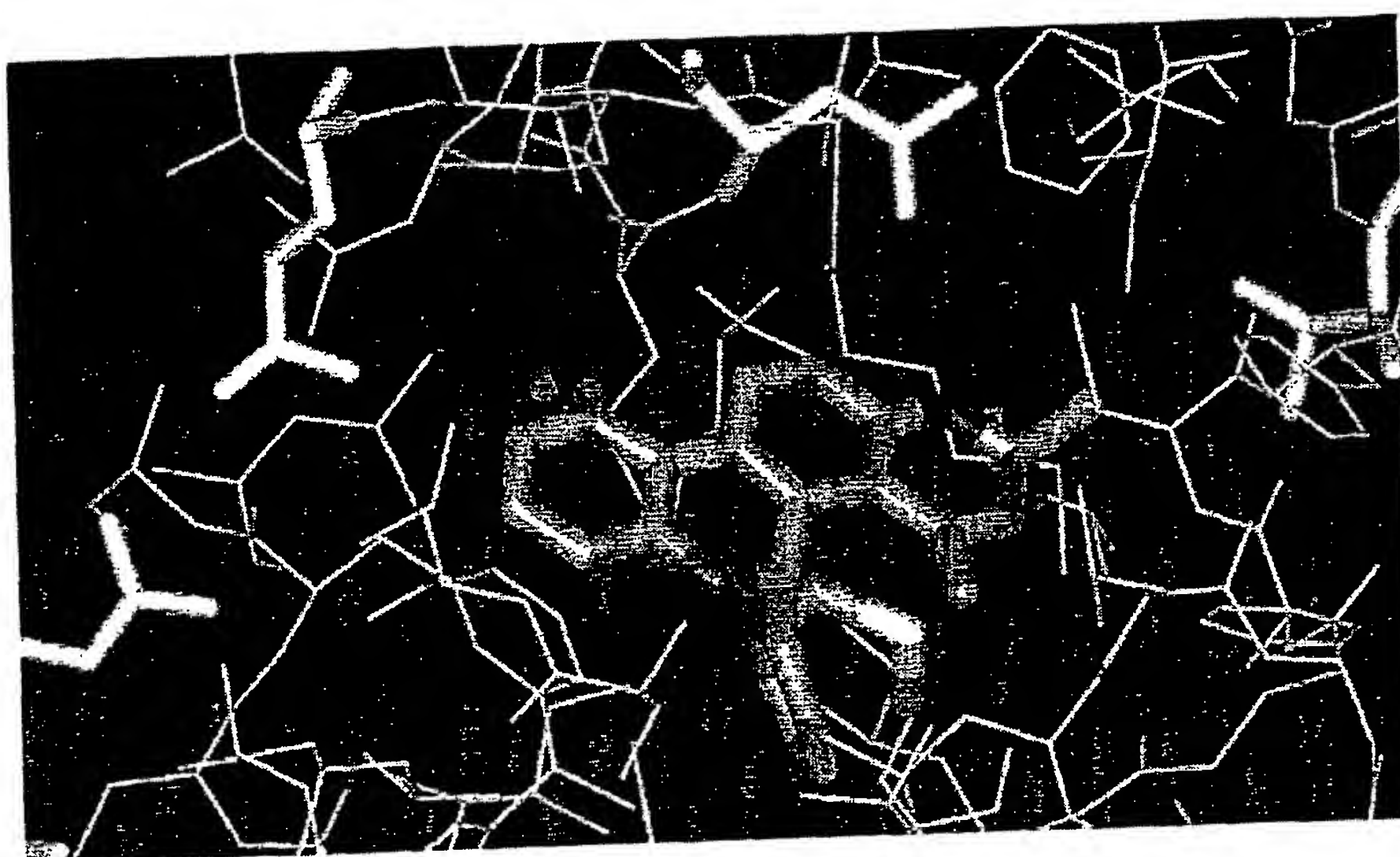


FIGURE 14

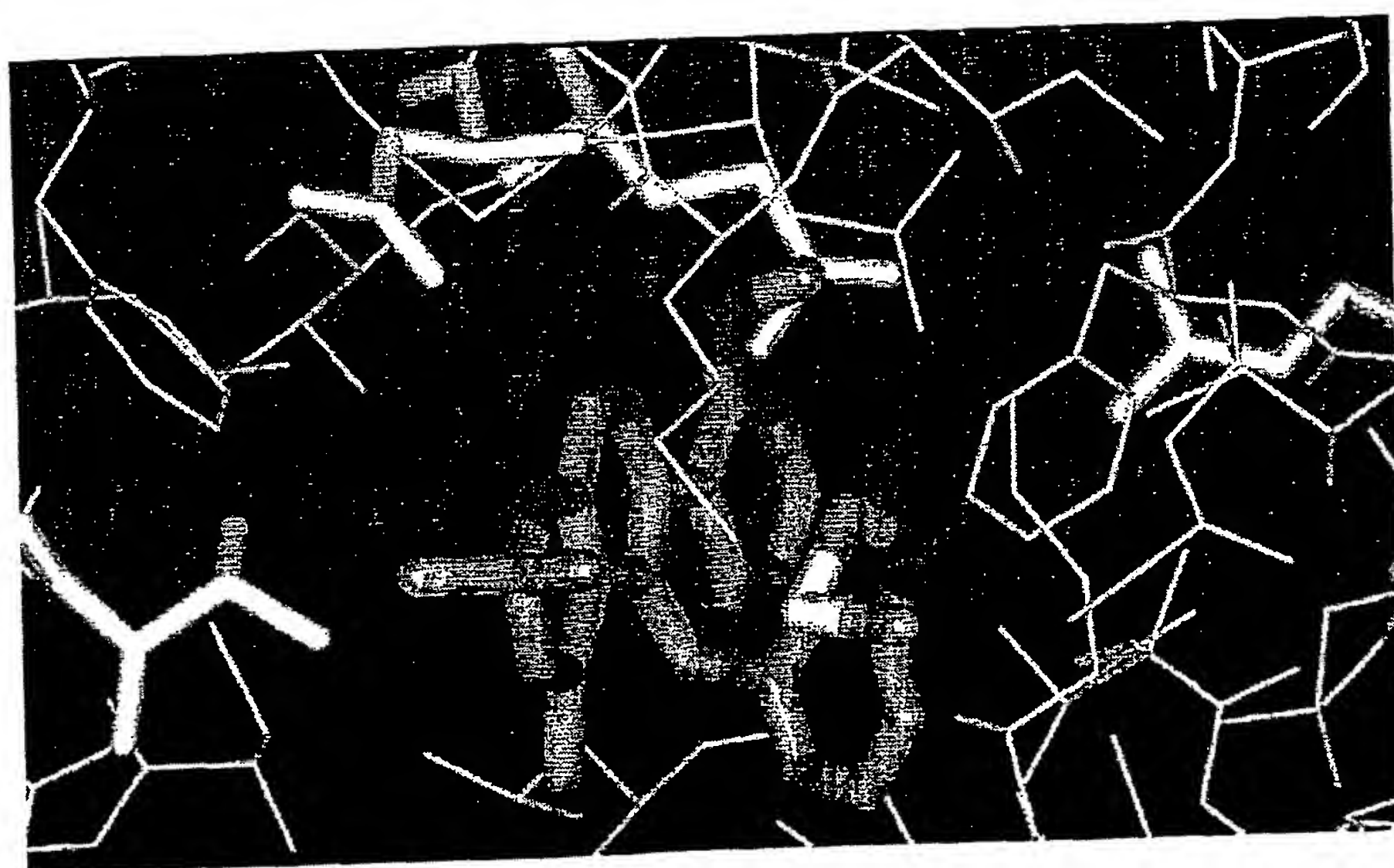


FIGURE 15

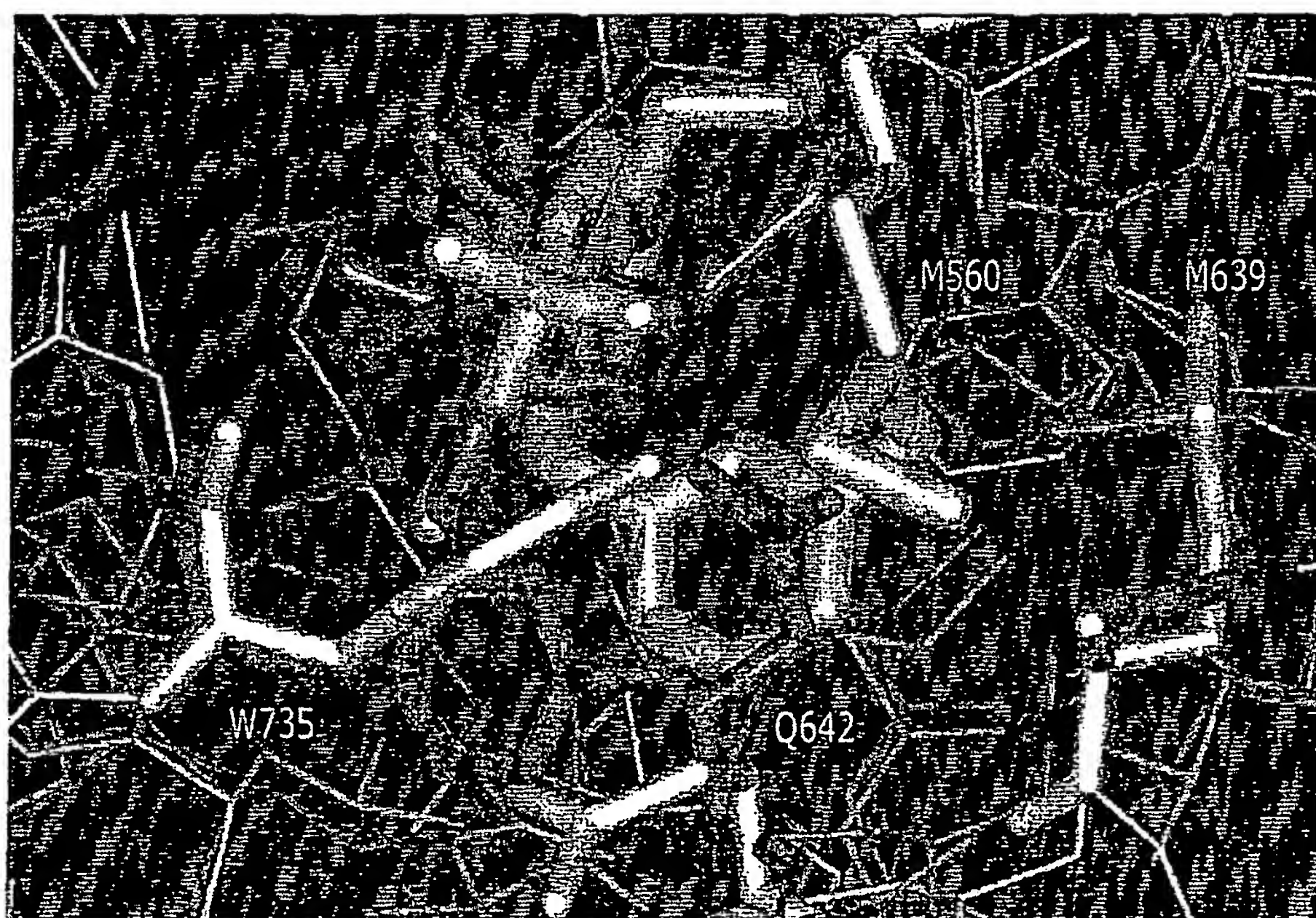


FIGURE 16

GR 527	QLTP	TLVSLLEVI	IEPEVLYAGYDSSVPDS	TWRIMTTL
MR 733	ALTP	SPVMVLENI	IEPEIVYAGYDSSKPD	TAENLLSTL
PR 682	QLIP	PLINLLMSI	IEPDVIYAGHDNTKPD	TSSSIITSL
AR 668	ECQP	IFLNVLEAI	IEPGVVCAGHDNNQPD	SFAALITSL
		helix-1		
GR 564	NMLGG	ROVIAAVKWAKA	I PGFRNLH	LDDQMTLLQYSW
MR 770	NRLAG	KQMIQVVKWAKV	L PGFKNL	PLEDQITLIQYSW
PR 719	NOLGER	QLLSVVKWSKSL	PGFRNLH	IDDQITLIQYSW
AR 705	NELGER	QLVHVVKWAKA	L PGFRNL	GVDDQMAVIQYSW
		helix-3	helix-3'	helix-4
GR 601	MSIMAF	ALGWR	SYROSSANLL	CFAPDLIINEQRM
MR 807	MCLSS	FALSWRSYKH	TNSQFLYFAPD	LVFNEEKMHQS
PR 756	MSIMV	FGLGWR	SYKHVSGQMLY	FAPDLILNEQRM
AR 742	MGIMV	FAMGWR	SFTNVNSRMLY	FAPDLVFNERYMHKS
		helix-5	beta-3	beta-4 helix-6
GR 638	CMYD	QCKHMLYVSSEL	HRLQVSYEEYL	LCMKTLLLLS
MR 844	AMYEL	CQGMHQISLQ	FVRLQLT	FEEYTIMKVLLLLST
PR 793	SFYS	LCLTMWQIPQ	EFVKLQVS	QEEFLCMKVLLLLNT
AR 779	RMYS	QCVRMRLHSQ	EFGLQIT	PQEFLLCMKALLFSI
		helix-7		helix-8
GR 675	VPKDGLKS	QELFDEIRMTYIKEL	GKAIVKREGNSSQN	
MR 881	IPKDGLKS	QAAFEEMRTNYIKEL	LRKMVTKCPNNSGQS	
PR 830	IPLEGLRS	QTQFEEMRSSYIRE	LKAIIGLRQKGVVSS	
AR 816	IPVDGLKN	QKFFDELRMNYIKEL	DRIJACKRKNPTSC	
		beta-5	helix-9	
GR 712	WQRFY	QLTKL	LDSDMHEVVENLLNYCF	QTEFLD-KTMSI
MR 918	WQRFY	QLTKL	LDSDMHDLVSDLLEFCFYTF	RESHALKV
PR 867	SQRFY	QLTKL	LDNLDLVKQLHLYCLNT	FIQSRALSV
AR 853	SRRFY	QLTKL	LDSDWQPIARELHQFT	FDLLIKSHMVS
			helix-10	
GR 748	EFP	EMLA	EITNQIPKYSNGN	IKKLLFHQK
MR 955	EFP	AMLVEI	ISDQLPKVESGNAK	PLYFHRK
PR 904	EFP	EMMSEVIAA	QLPKILAGMVKP	LLFHKK
AR 890	DFP	EMMAEI	ISVQVPKILSGKVKP	IYFHTQ
		helix-AF	beta-6	

FIGURE 17

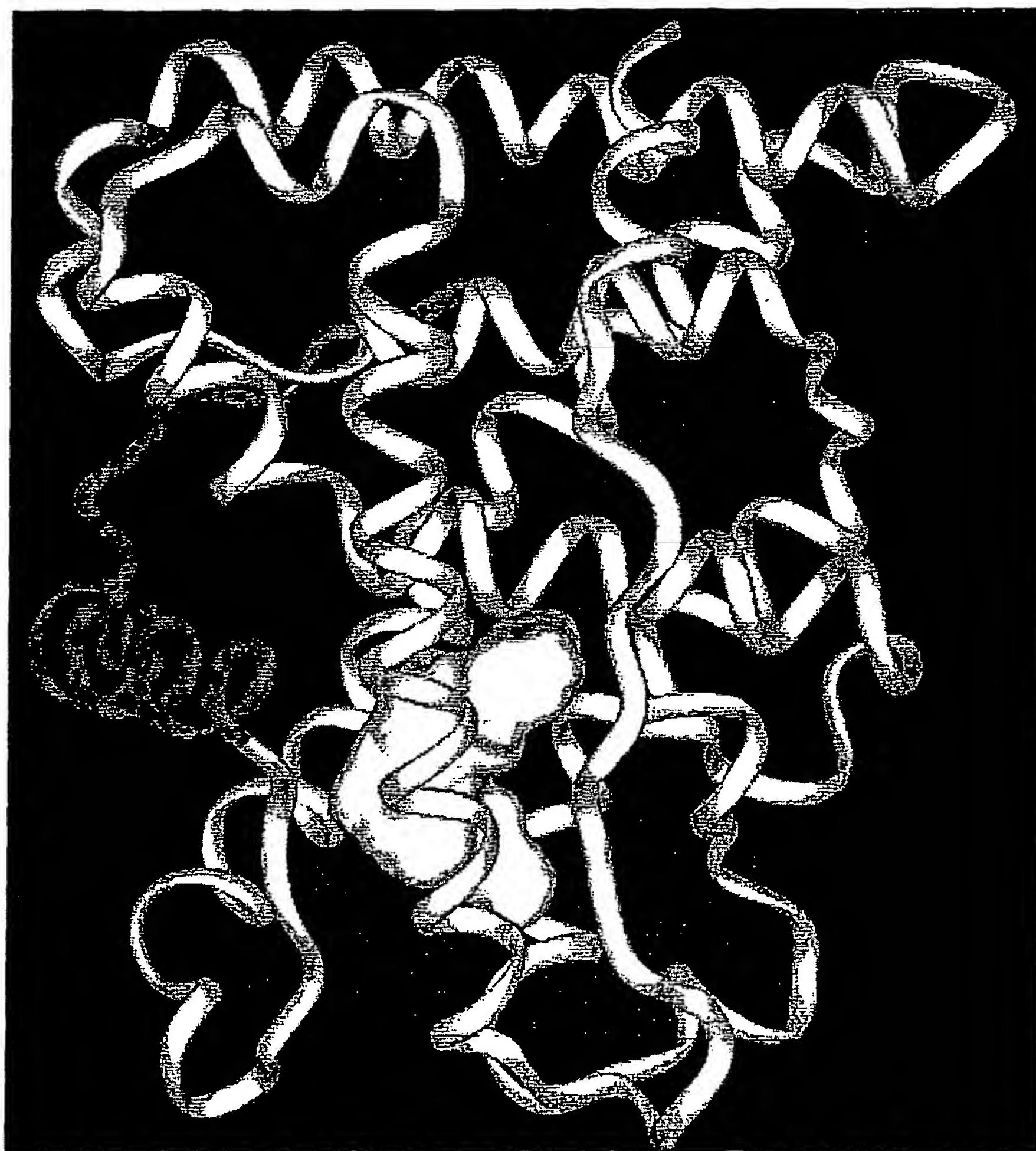


FIGURE 18A

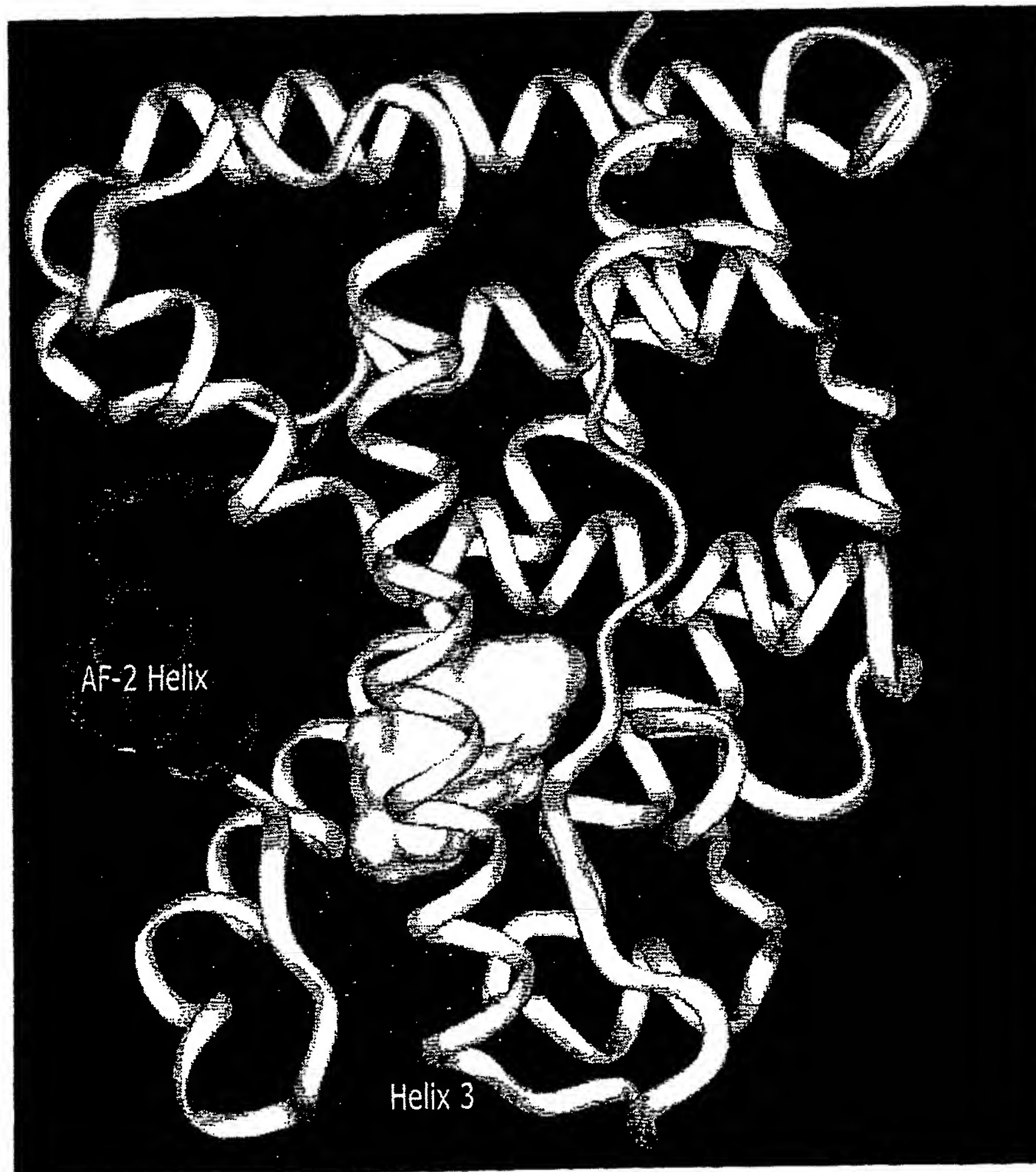


FIGURE 18B

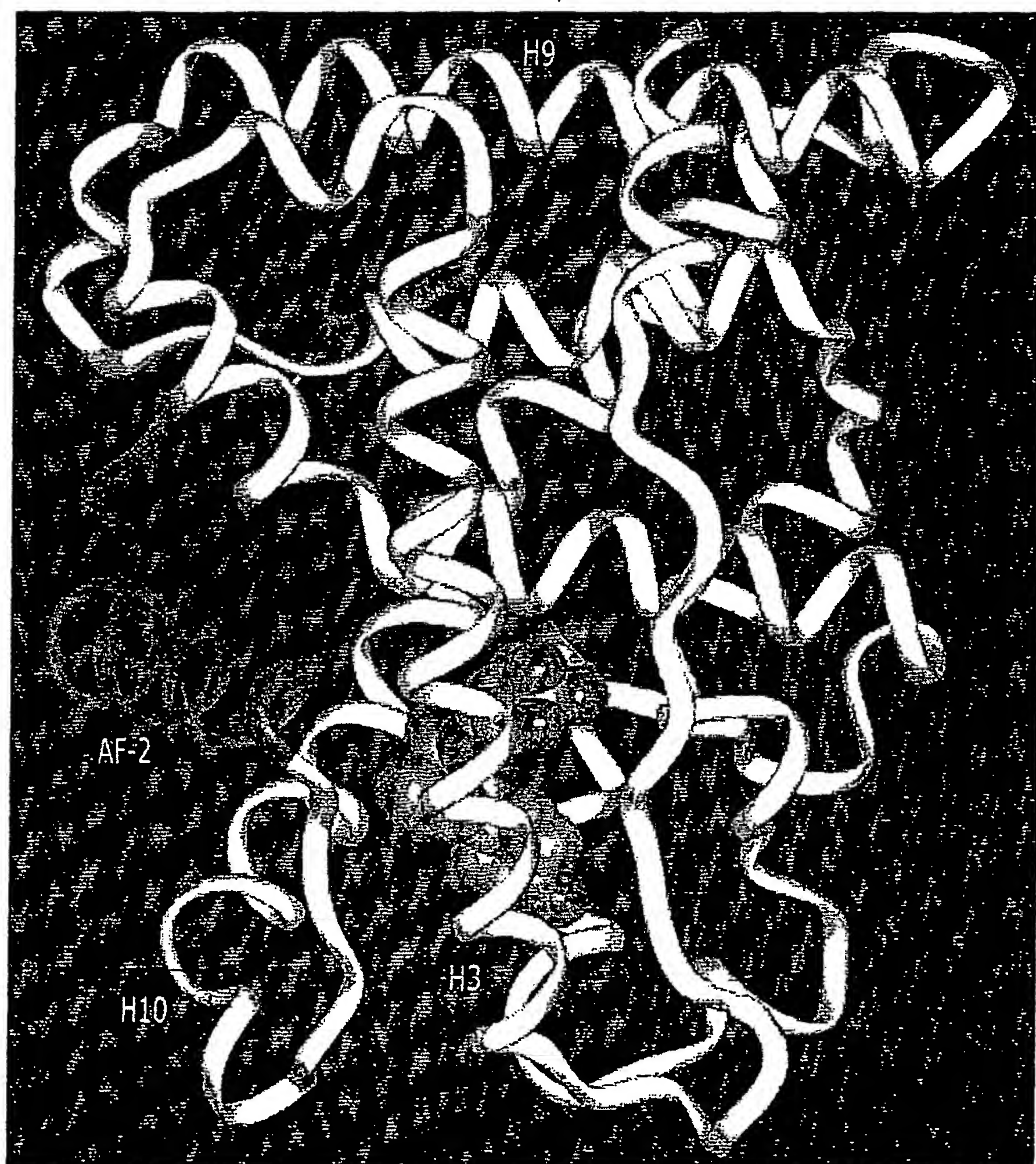


FIGURE 19

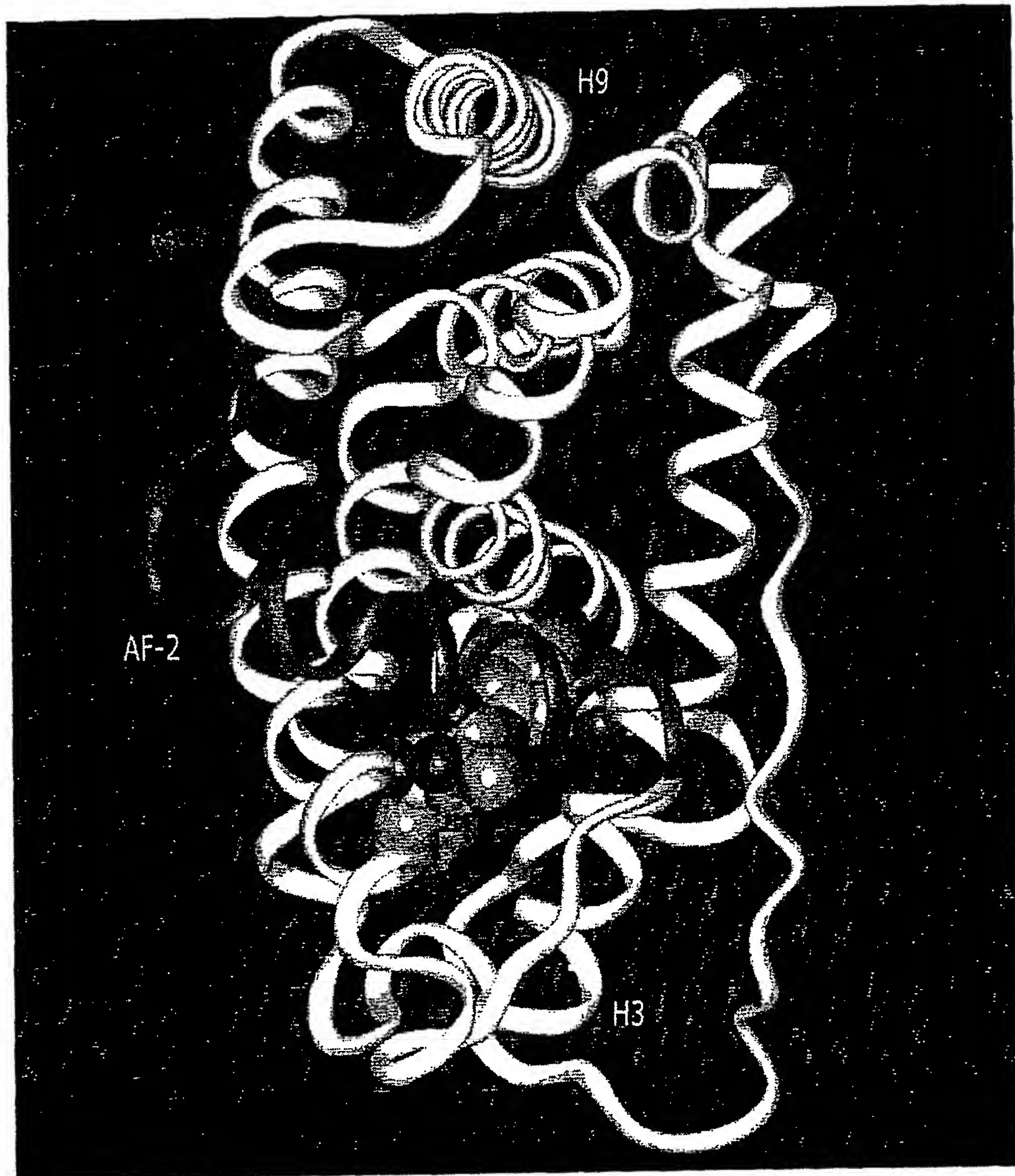


FIGURE 20

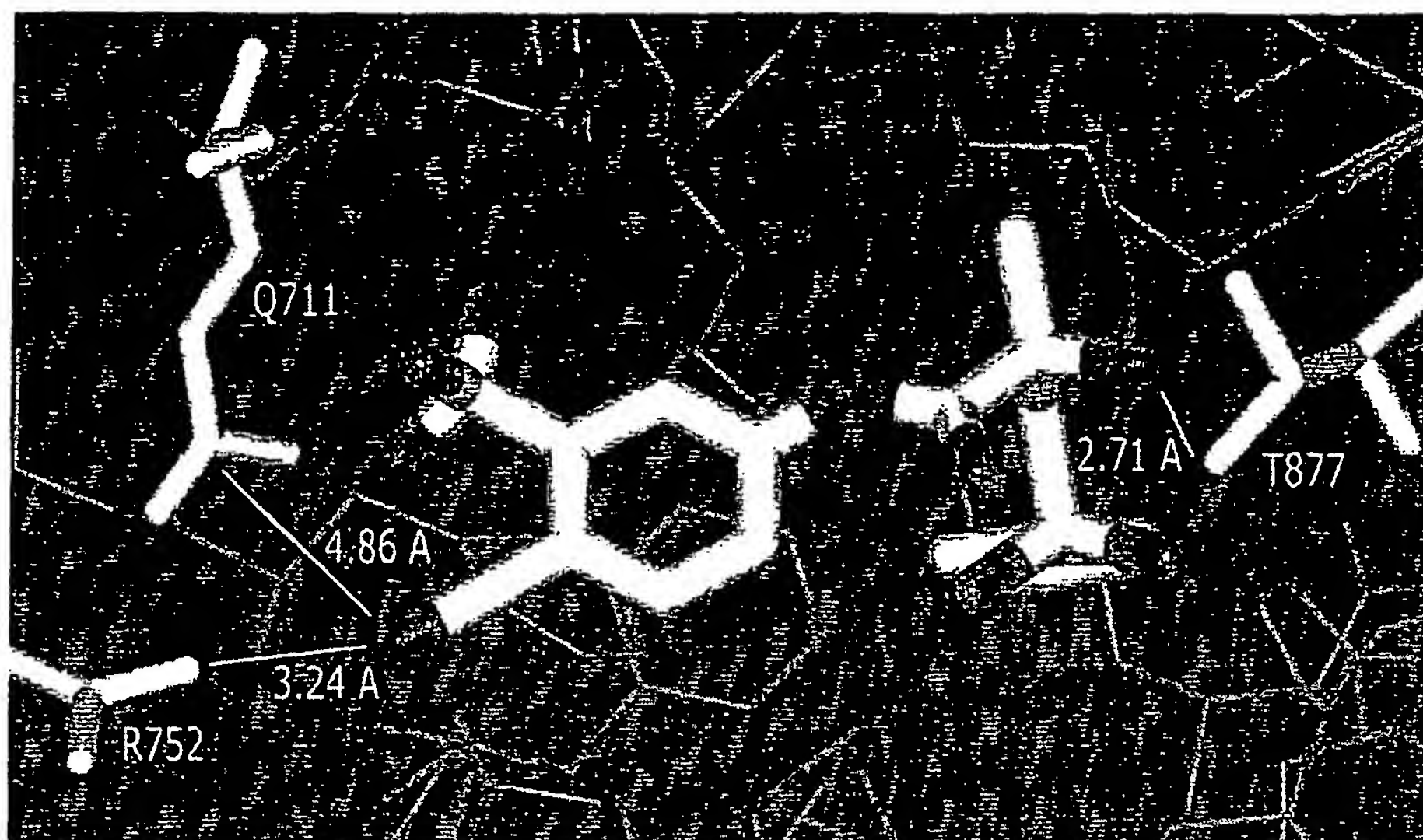


FIGURE 21

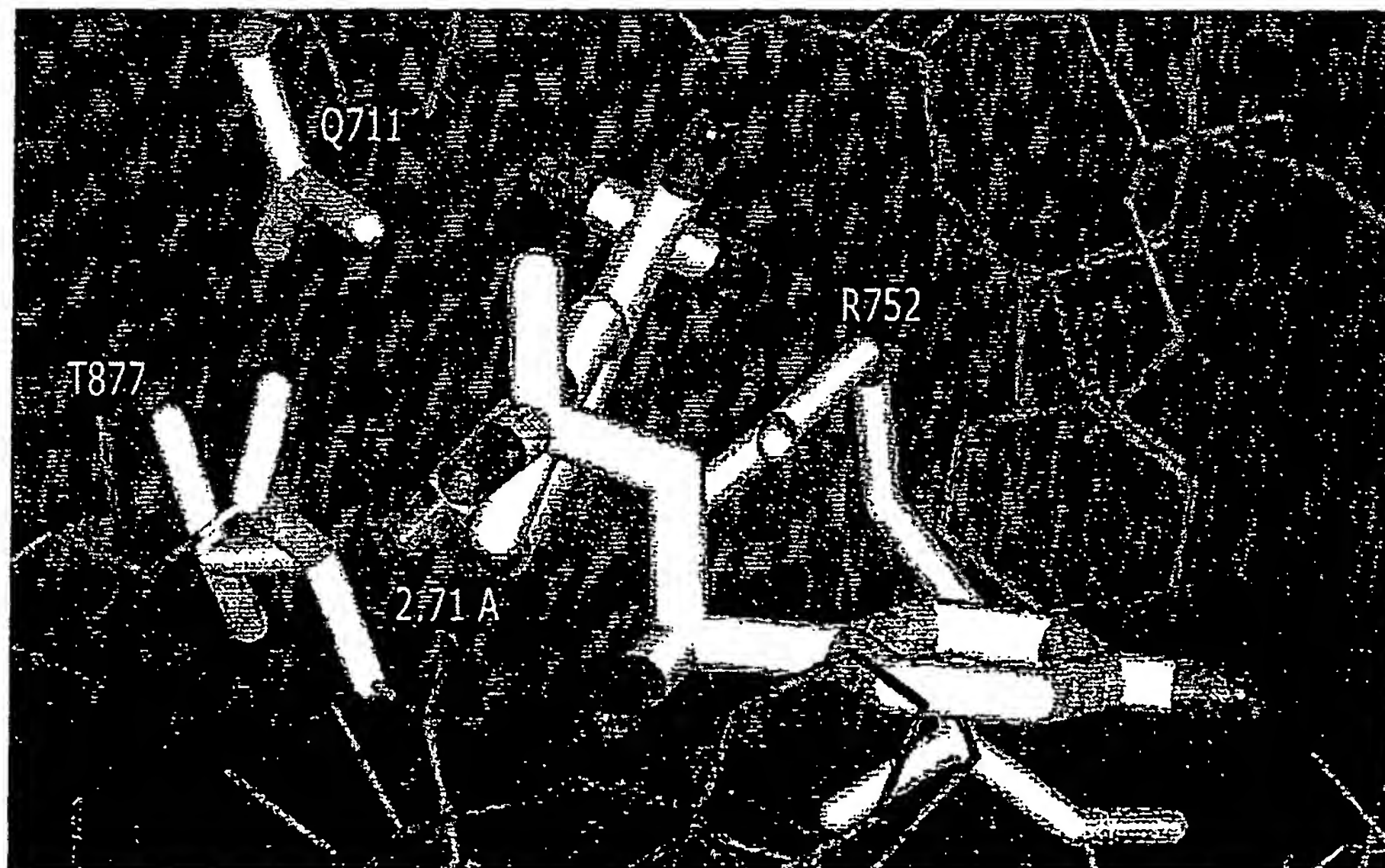


FIGURE 22

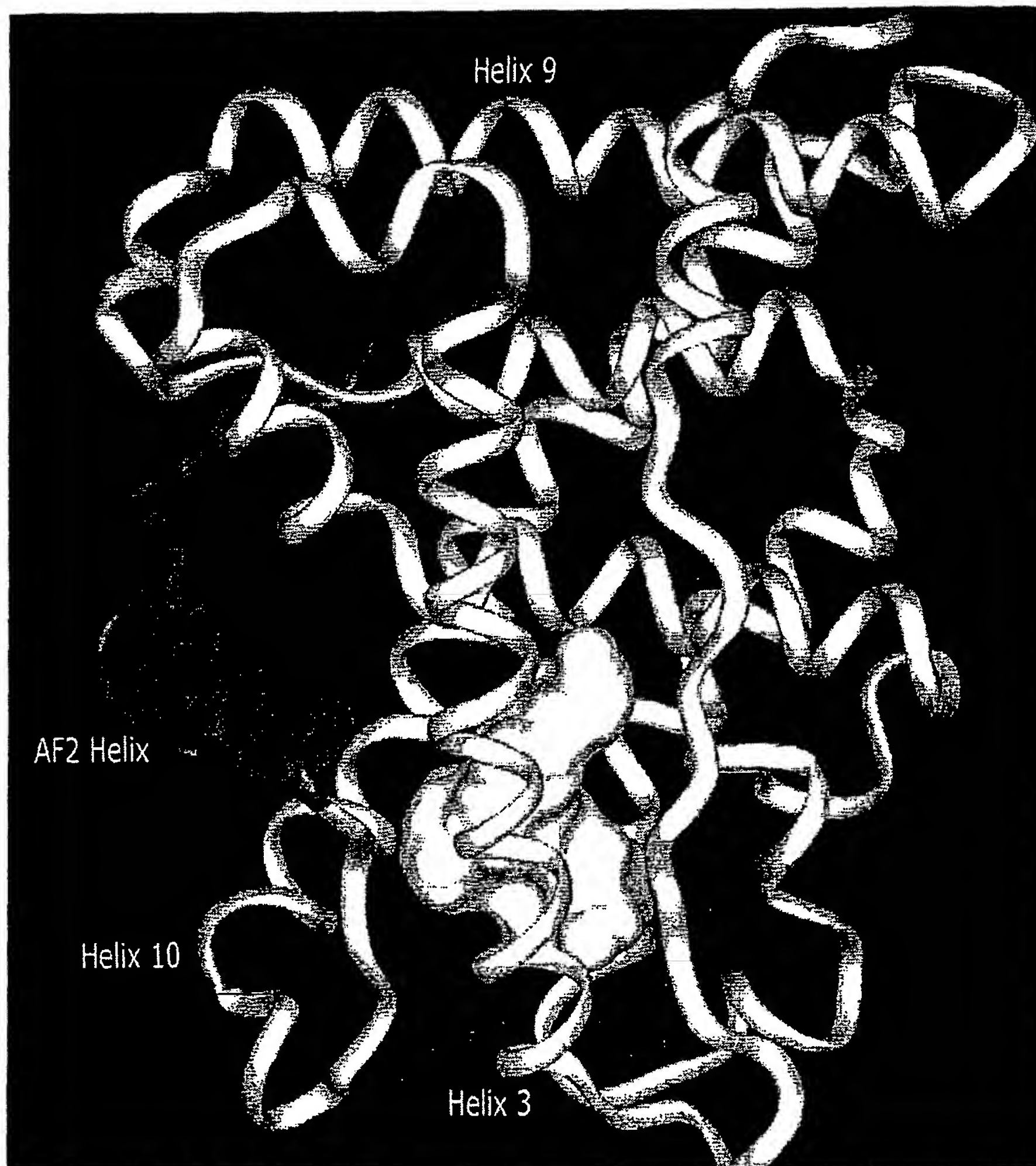


FIGURE 23A

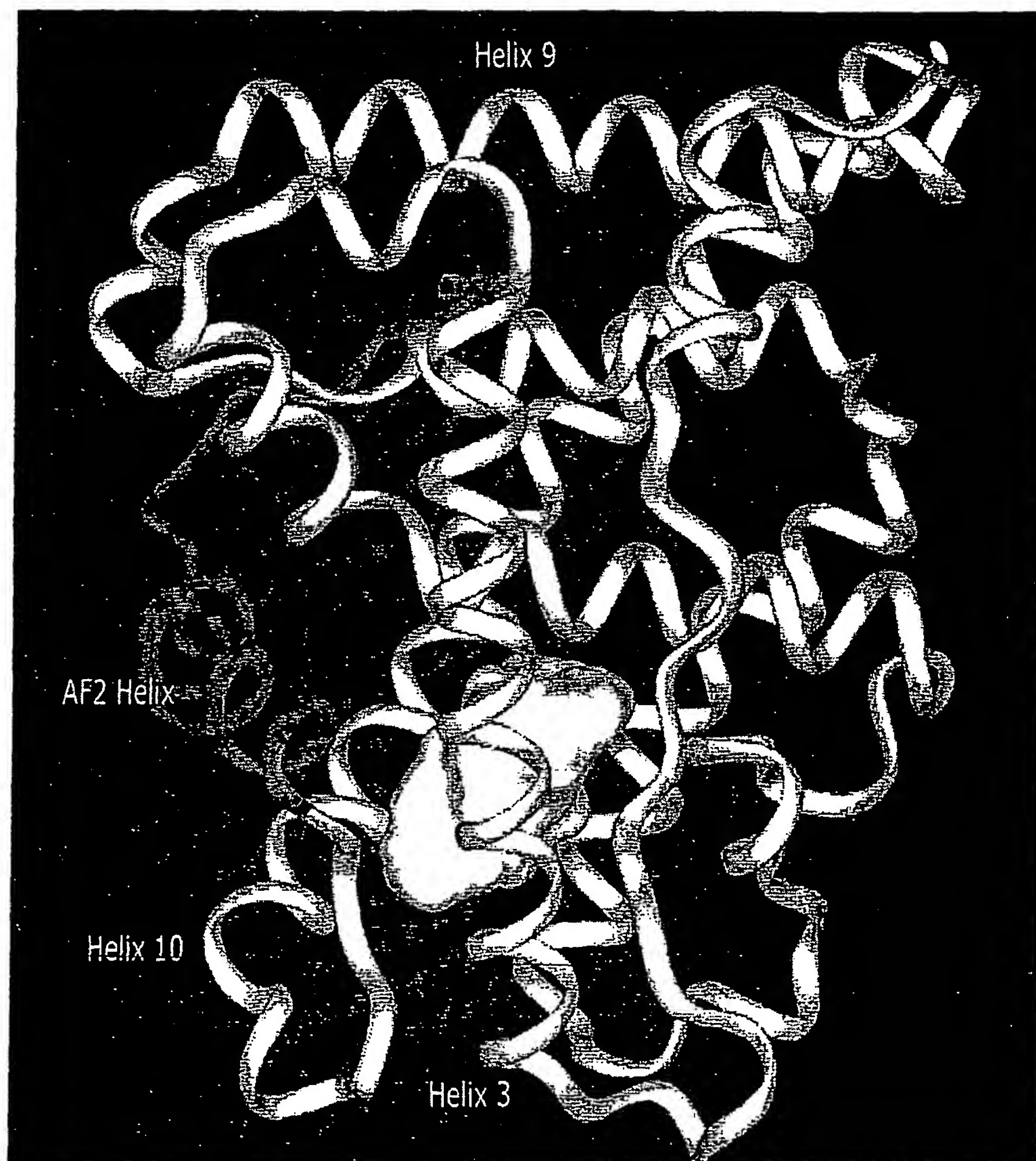


FIGURE 23B

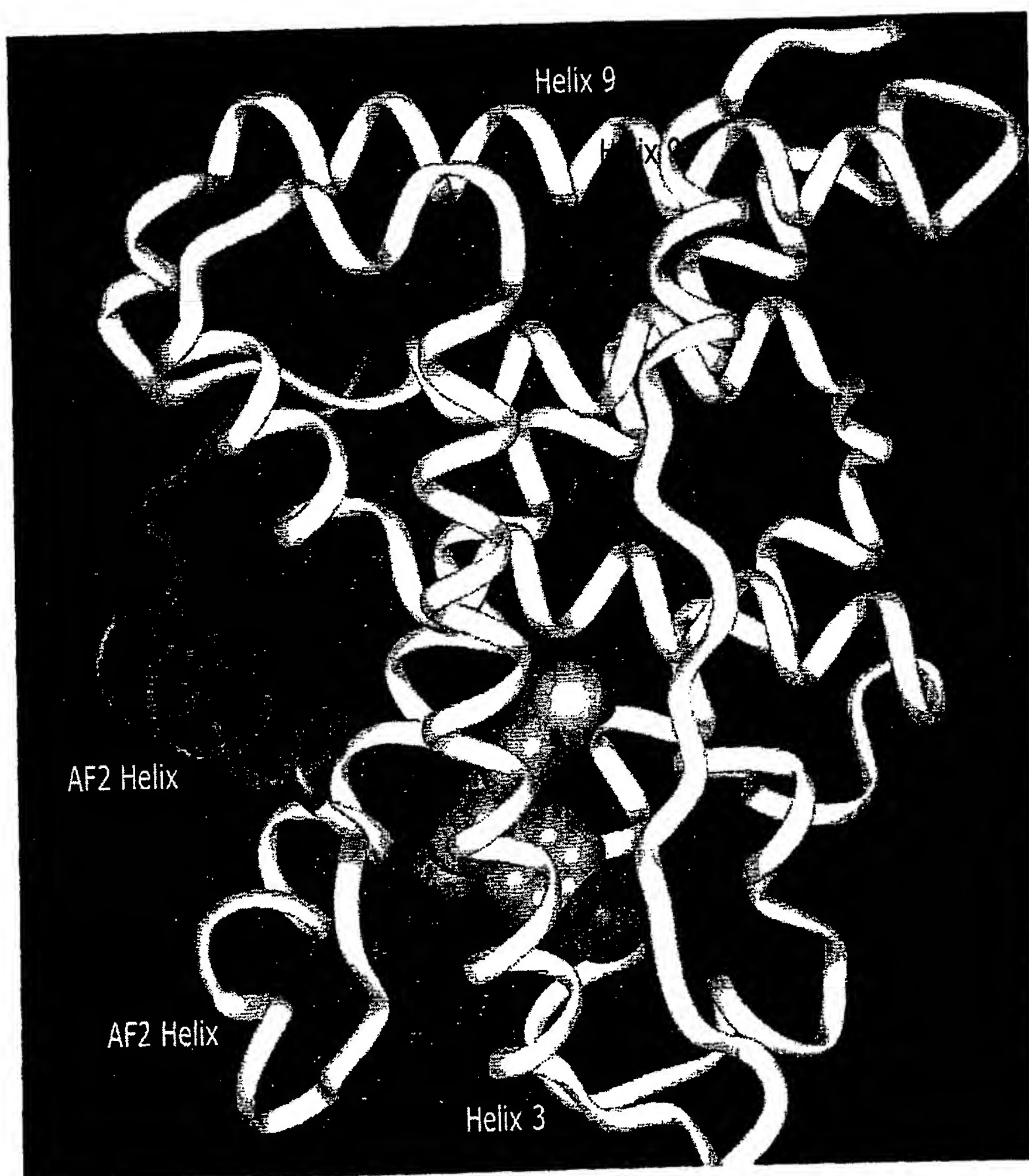


FIGURE 24

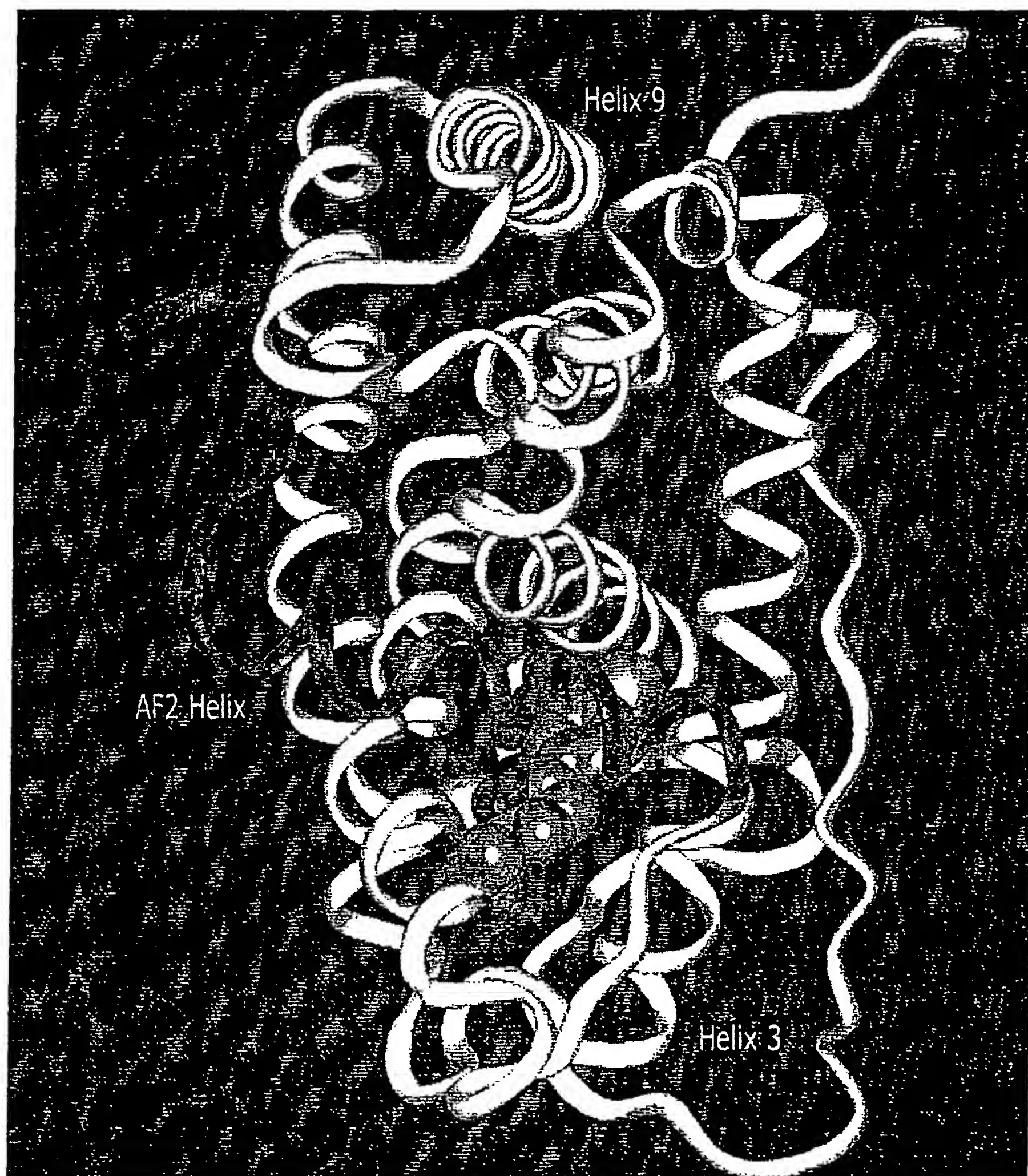


FIGURE 25

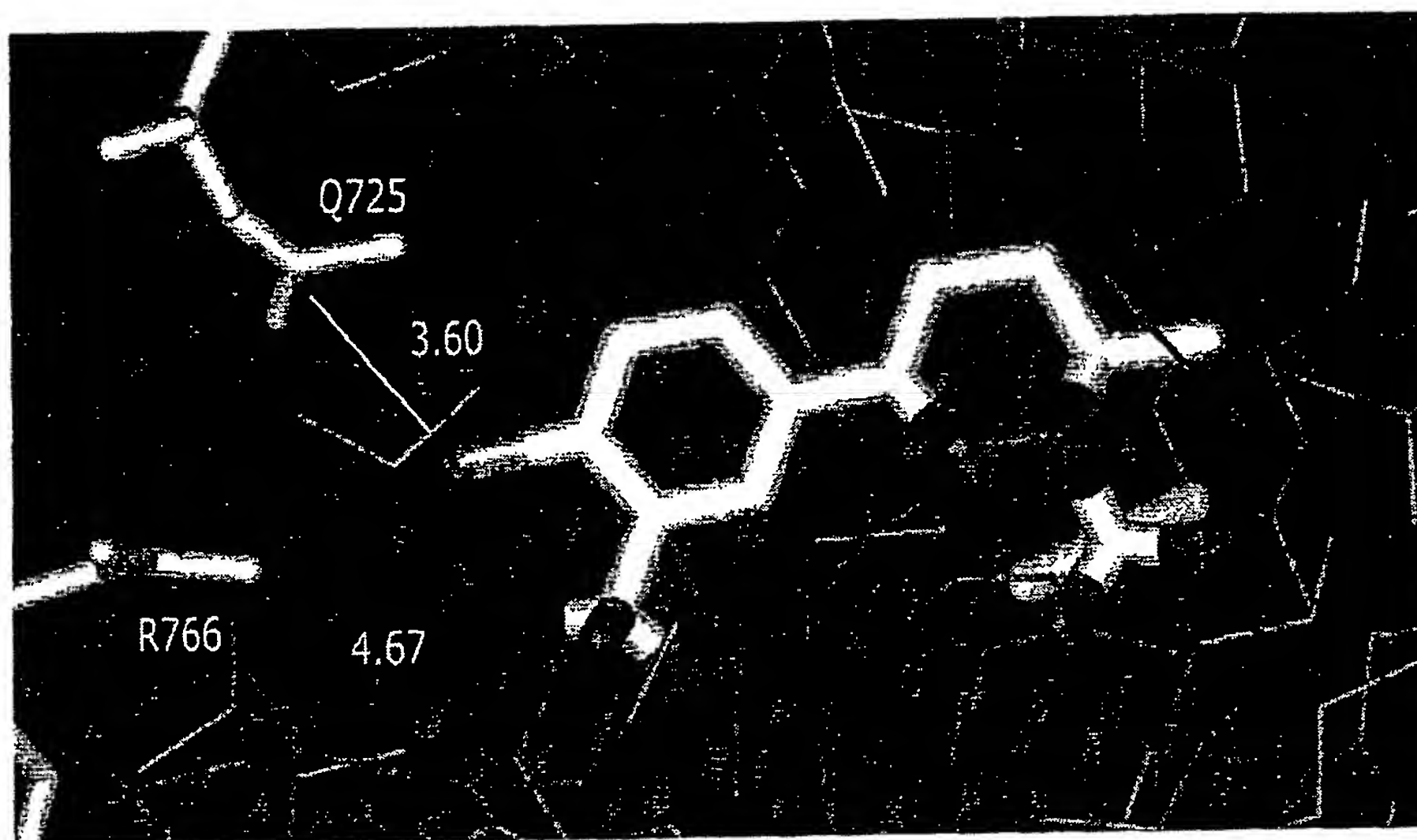


FIGURE 26

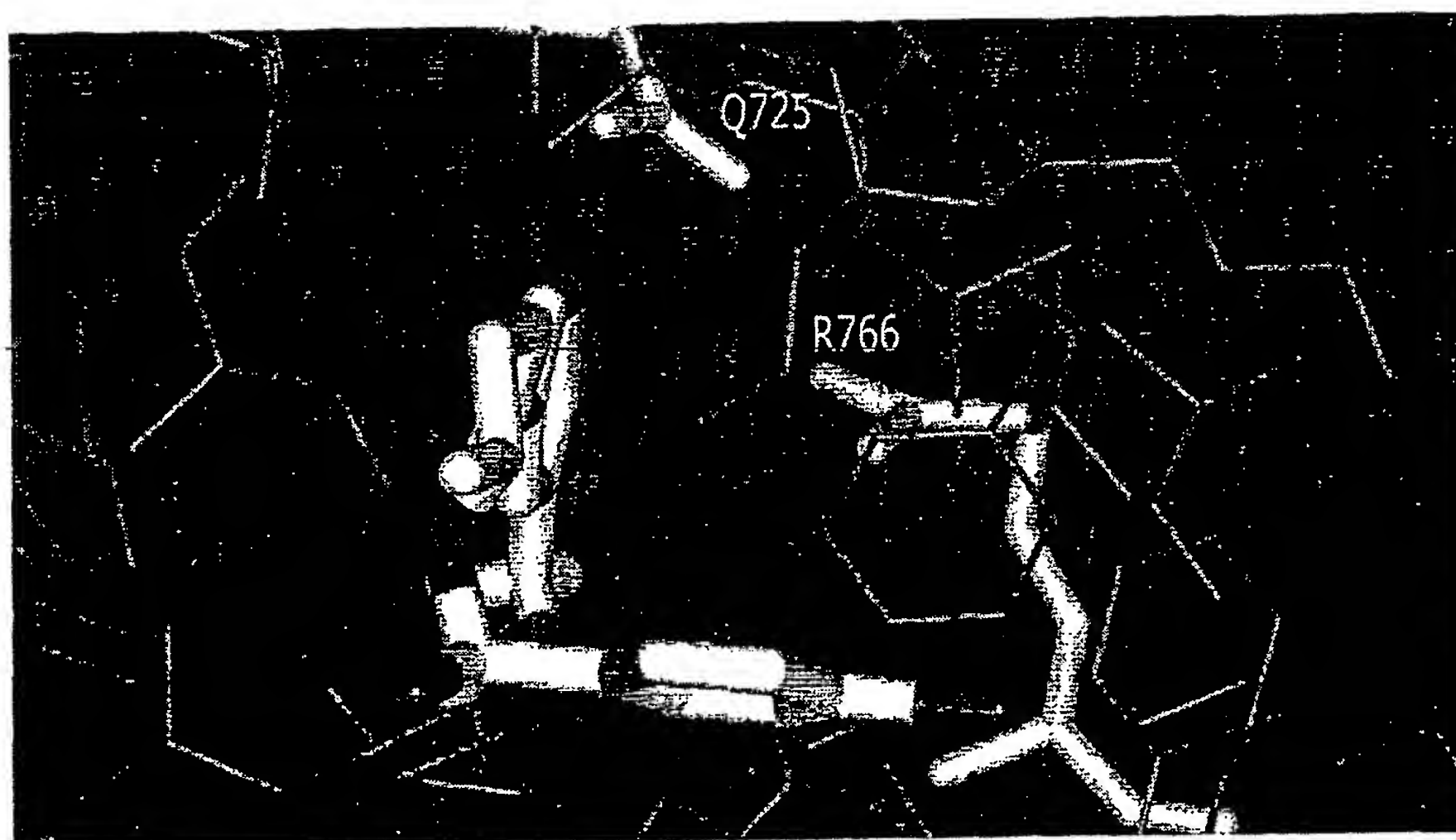


FIGURE 27

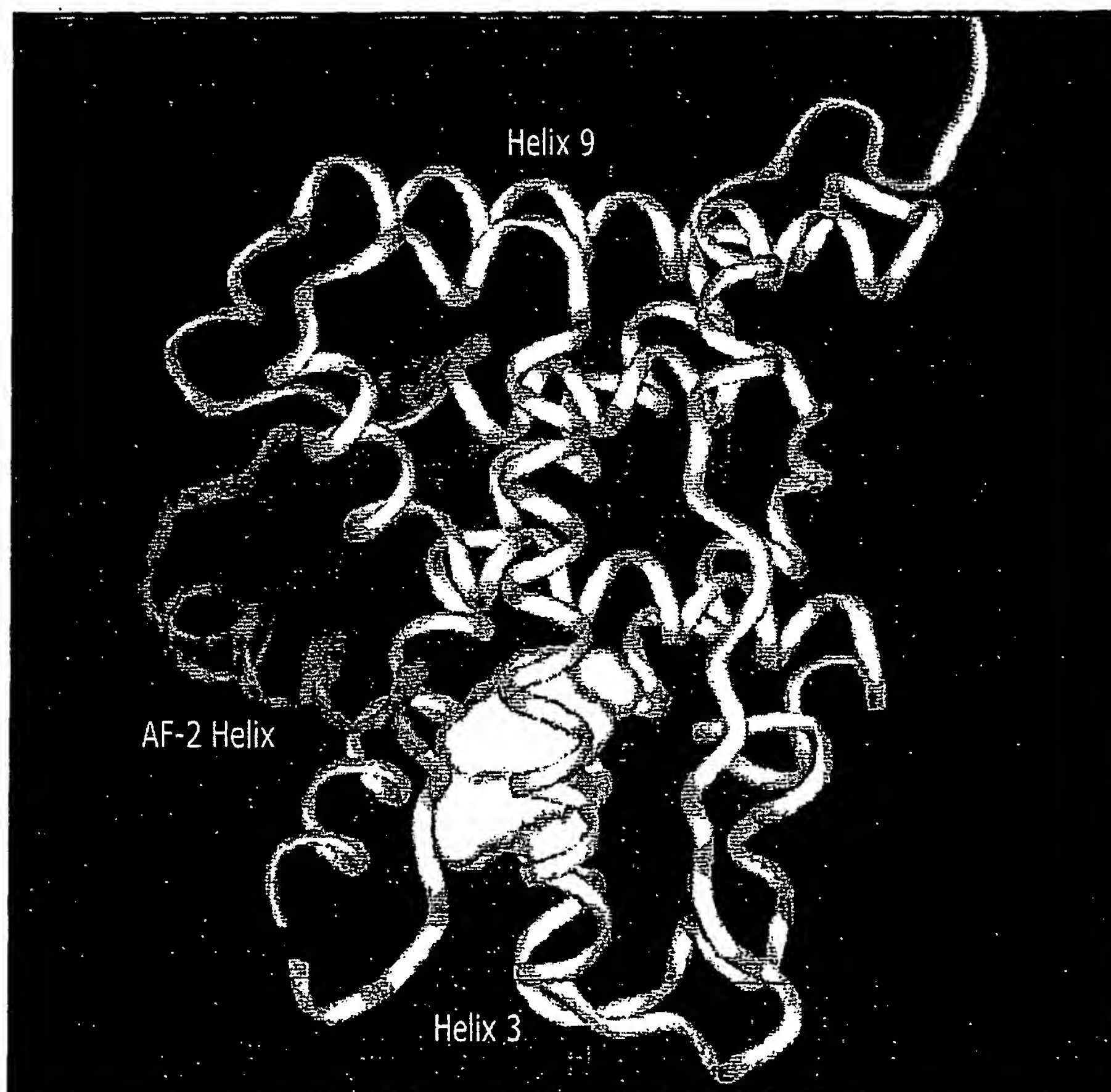


FIGURE 28A

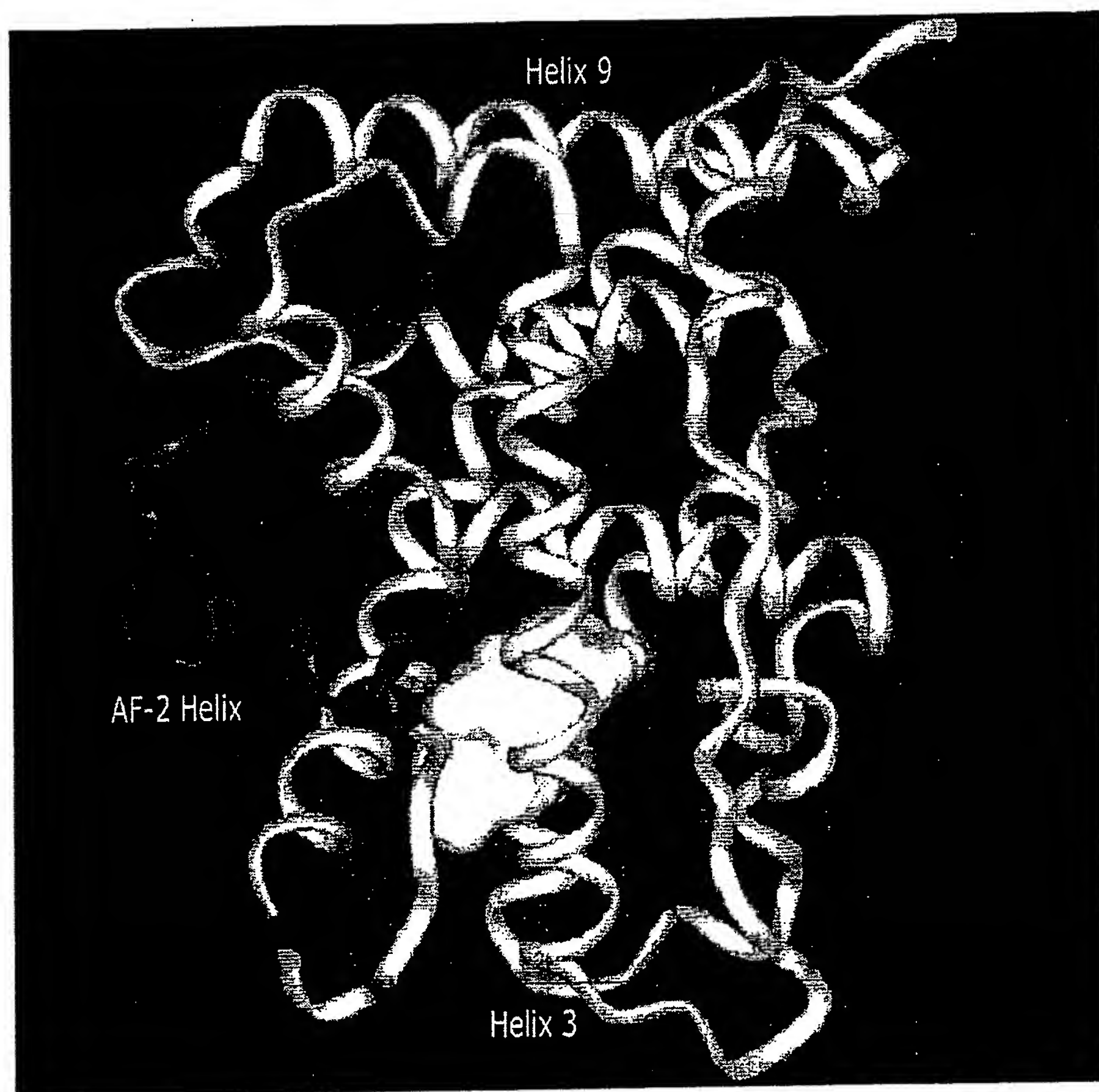


FIGURE 28B



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DOCUMENTS CONSIDERED TO BE RELEVANT			
Category	Citation of document with indication, where appropriate, of relevant passages	Relevant to claim	CLASSIFICATION OF THE APPLICATION (Int.Cl.7)
A	HOLLENBERG S M ET AL: "PRIMARY STRUCTURE AND EXPRESSION OF A FUNCTIONAL HUMAN GLUCOCORTICOID RECEPTOR CDNA" NATURE, MACMILLAN JOURNALS LTD. LONDON, GB, vol. 318, 19 December 1985 (1985-12-19), pages 635-641, XP000611470 ISSN: 0028-0836 * the whole document *	1-47	C07K14/72 G06F19/00
A	STEVENS R C: "High-throughput protein crystallization" CURRENT OPINION IN STRUCTURAL BIOLOGY, CURRENT BIOLOGY LTD., LONDON, GB, vol. 10, no. 5, October 2000 (2000-10), pages 558-563, XP002208529 ISSN: 0959-440X * the whole document *	1-47	
A	WILLIAMS SHAWN P ET AL: "Atomic structure of progesterone complexed with its receptor" NATURE, MACMILLAN JOURNALS LTD. LONDON, GB, vol. 393, no. 6683, 28 May 1998 (1998-05-28), pages 392-396, XP002173773 ISSN: 0028-0836 * the whole document *	1-47	TECHNICAL FIELDS SEARCHED (Int.Cl.7) C07K G06F
A	WO 02 36606 A (MATRIX THERAPEUTICS LTD ;MIEL HUGHES JEAN PIERRE (GB); RAY DAVID W) 10 May 2002 (2002-05-10) * examples 1-3 *	1-47	
The present search report has been drawn up for all claims			
Place of search MUNICH		Date of completion of the search 21 August 2003	Examiner Petri, B
<p>CATEGORY OF CITED DOCUMENTS</p> <p>X: particularly relevant if taken alone Y: particularly relevant if combined with another document of the same category A: technological background O: non-written disclosure P: intermediate document</p> <p>T: theory or principle underlying the invention E: earlier patent document, but published on, or after the filing date D: document cited in the application L: document cited for other reasons &: member of the same patent family, corresponding document</p>			

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DOCUMENTS CONSIDERED TO BE RELEVANT			
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A	<p>DEY R ET AL: "Homology modelling of the ligand-binding domain of glucocorticoid receptor: binding site interactions with cortisol and corticosterone"</p> <p>PROTEIN ENGINEERING, OXFORD UNIVERSITY PRESS, SURREY, GB, vol. 14, no. 8, 2001, pages 565-571, XP002964886 ISSN: 0269-2139 * the whole document *</p>	1-47	
P,X	<p>WO 03 015692 A (APOLITO CHRISTOPHER J ; LAMBERT MILLARD H III (US); SMITHKLINE BEEC) 27 February 2003 (2003-02-27) * the whole document *</p>	1-47	
P,X	<p>BLED SOE R K ET AL: "Crystal structure of the glucocorticoid receptor ligand binding domain reveals a novel mode of receptor dimerization and coactivator recognition"</p> <p>CELL, CELL PRESS, CAMBRIDGE, NA, US, vol. 110, 12 July 2002 (2002-07-12), pages 93-105, XP002964887 ISSN: 0092-8674 * the whole document *</p>	1-47	
A	<p>WO 00 52050 A (GREENIDGE PAULETTE ; GILLNER MIKAEL (SE); KAROBIO AB (SE)) 8 September 2000 (2000-09-08) * the whole document *</p>	1-47	
The present search report has been drawn up for all claims			<p>TECHNICAL FIELDS SEARCHED (Int.Cl.7)</p>
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Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 0236606 A	10-05-2002	AU 1076802 A	15-05-2002
		CA 2427569 A1	10-05-2002
		EP 1335928 A1	20-08-2003
		WO 0236606 A1	10-05-2002
WO 03015692 A	27-02-2003	WO 03015692 A2	27-02-2003
WO 0052050 A	08-09-2000	AU 2818200 A	21-09-2000
		WO 0052050 A2	08-09-2000

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